

SEP 0 9 2002 **TECH CENTER 1600/2900**

FIG. 1

			ACOM						
			Type	Res.		<u>x</u>	<u>Y</u>	<u>z</u>	
	ATOM	1	С	GLY	1	69.326	51.394	17.320	
183	ATCM	2	0	GLY	1	69.833	51.813	16.277	1
4	ATOM	3	N	GLY	1	70.959	52.760	18.620	
IG. SUBCLASS	ATOM	4	CA	GLY	1	70.031	51.571	18.653	1
의물	ATOM	5	N	ILE	2	68.153	50.776	17.347	1
14	ATOM	6	CA	ILE	2	67.404	50.567	16.121	1
CD AS	ATOM	7	CB	ILE	2	66.717	49.195	16.121	
9.9	ATOM	8	CG2	ILE `	2	65.743	49.071	14.958	1
p	ATOM	9	CG1	ILE	2	67.788	48.104	16.055	1
1E 31	ATOM	10	CD1	ILE	2	67.235	46.714	16.136	1
APPROVED BY DRAFTSMAN	ATOM	11	C	ILE	2	66.379	51.671	15.959	1
15 \$1	ATOM	12	0	ILE	2	65.635	51.988	16.893	1
1, 5	ATOM	13	N	TYR	3	66.358	52.282	14.781	1
	ATOM	14	CA	TYR	3	65.407	53.355	14.515	1
	ATOM	15	CB	TYR	3	65.923	54.291	13.420	1
	ATOM	16	CG	TYR	3	64.952	55.408	13.420	1
	ATOM	17	CD1	TYR	3	64.870	56.552	13.887	1
	ATOM	18	CE1	TYR	3	63.950	57.569	13.608	1
	ATOM	19	CD2	TYR	3	64.090	55.307	11.999	1
	ATOM	20	CE2	TYR	3	63.166	56.313	11.709	1
	ATOM	21	CZ	TYR	3	63.102	57.444	12.517	1
	ATOM	22	OH	TYR	3	62.204	58.454	12.225	1
	ATOM	23	С	TYR	3	64.075	52.766	14.068	1
	ATOM	24	0	TYR	3	63.022	53.193	14.517	1
	ATOM	25	N	GLY	4	64.130	51.792	13.166	1
	ATOM	26	CA	GLY	4	62.909	51.182	12.672	í
	ATOM	27	С	GLY	4	63.216	49.984	11.799	1
	ATOM	28	0	GLY	4	64.354	49.800	11.371	1
	ATOM	29	N	ILE	5	62.211	49.145	11.562	1.
	ATOM	30	CA	ILE	5	62.402	47.985	10.704	1
	30014							20.704	Ι.

		Ato	m						
		Typ	e Res		<u>x</u>	Y	z	OCC B	MOL
ATOM	1	С	GLY	1	69.326	51.394	17.320		
ATOM	2	0	GLY	1	69.833	51.813	16.277	1.00 31.75	CPS1
ATOM	3	N	GLY	1	70.959	52.760	18.620	1.00 31.77	CPS1
ATOM	4	CA	GLY	1	70.031	51.571	18.653	1.00 35.87	CPS1
ATOM	5	N	ILE	2	68.153	50.776	17.347	1.00 32.48	CPS1
ATOM	6	CA	ILE	2	67.404	50.567	16.121	1.00 26.25	CPS1
ATOM	7	CB	ILE	. 2	66.717	49.195	16.134	1.00 25.90	CPS1
ATOM ATOM	8		2 ILE	2	65.743	49.071	14.958	1.00 25.20	CPS1 CPS1
ATOM	9		LILE	2	67.788	48.104	16.055	1.00 28.68	CPS1
ATOM	10 11	CD:	LILE	2	67.235	46.714	16.136	1.00 29.70	CPS1
ATOM	12	0	ILE	2	66.379	51.671	15.959	1.00 24.77	CPS1
ATOM	13	и	TYR	2	65.635	51.988	16.893	1.00 24.24	CPS1
ATOM	14	CA	TYR	3 3	66.358	52.282	14.781	1.00 23.49	CPS1
ATOM	15	CB	TYR	3	65.407	53.355	14.515	1.00 23.75	CPS1
ATOM	16	CG	TYR	3	65.923	54.291	13.420	1.00 25.80	CPS1
ATOM	17		. TYR	3	64.952 64.870	55.408	13.087	1.00 28.36	CPS1
ATOM	18	CEI		3	63.950	56.552 57.569	13.887	1.00 30.78	CPS1
ATOM	19	CD2		3	64.090	55.307	13.608	1.00 33.13	CPS1
ATOM	20	CE2		3	63.166	56.313	11.999	1.00 29.71	CPS1
ATOM	21	cz	TYR	3	63.102	57.444	12.517	1.00 32.64	CPS1
ATOM	22	OH	TYR	3	62.204	58.454	12.225	1.00 34.23 1.00 36.12	CPS1
ATOM	23	С	TYR	3	64.075	52.766	14.068	1.00 23.33	CPS1
ATOM	24	0	TYR	3	63.022	53.193	14.517	1.00 24.16	CPS1
ATOM	25	N	GLY	4	64.130	51.792	13.166	1.00 21.11	CPS1 CPS1
ATOM	26	CA	GLY	4	62.909	51.182	12.672	1.00 20.13	CPS1
ATOM	27	С	GLY	4	63.216	49.984	11.799	1.00 19.67	CPS1
ATOM	28	0	GLY	4	64.354	49.800	11.371	1.00 18.21	CPS1
ATOM	29	N	ILE	5	62.211	49.145	11.562	1.00 18.70	CPS1
ATOM	30	CA	ILE	5	62.402	47.985	10.704	1.00 17.69	CPS1
ATOM ATOM	31 32	CB	ILE	5	62.470	46.666	11.510	1.00 18.45	CPS1
ATOM	32		ILE	5	63.538	46.799	12.610	1.00 17.74	CPS1
ATOM	34		ILE	5 5	61.103	46.329	12.127	1.00 17.47	CPS1
ATOM	35	C	ILE	5	61.097	44.956	12.830	1.00 18.74	CPS1
ATOM	36	ō	ILE	5	61.225	47.936	9.736	1.00 17.16	CPS1
ATOM	37	N	GLY	6	60.170 61.414	48.525	10.001	1.00 16.88	CPS1
ATOM	38	CA	GLY	6	60.353	47.248	8.616	1.00 16.81	CPS1
ATOM	39	c	GLY	6	60.398	47.163 45.846	7.632	1.00 16.27	CPS1
ATOM	40	ō	GLY	6	61.468	45.303	6.893 6.623	1.00 17.21 1.00 17.76	CPS1
ATOM	41	N	LEU	7	59.220	45.345	6.555	1.00 17.76	CPS1
ATOM	42	CA	LEU	7	59.085	44.080	5.858	1.00 17.08	CPS1 CPS1
ATOM	43	CB	LEU	7	58.631	43.006	6.857	1.00 18.52	CPS1
ATOM	44	CG	LEU	7	58.266	41.643	6.270	1.00 18.46	CPS1
ATOM	45		LEU	7	59.552	40.921	5.800	1.00 18.60	CPS1
ATOM	46		LEU	7	57.546	40.825	7.342	1.00 19.42	CPS1
ATOM	47	C	LEU	7	58.025	44.246	4.780	1.00 18.80	CPS1
ATOM	48	0	LEU	7	57.036	44.935	4.988	1.00 19.60	CPS1
ATOM ATOM	49	N	ASP	8	58.240	43.632	3.623	1.00 18.18	CPS1
	50	CA	ASP	8	57.256	43.693	2.558	1.00 18.85	CPS1
ATOM ATOM	51	CB	ASP	8	57.514	44.898	1.629	1.00 20.11	CPS1
ATOM	52 53	CG	ASP	8	56.550	44.927	0.447	1.00 21.89	CPS1
ATOM	54	OD1		8	56.853	44.324	-0.600	1.00 24.47	CPS1
ATOM	55	OD2 C	ASP	8	55.471	45.524	0.585	1.00 25.95	CPS1
ATOM	56	0	ASP	8	57.293	42.422	1.723	1.00 18.97	CPS1
	50	•	nar	8	58.353	41.856	1.486	1.00 19.21	CPS1



SEP 0 9 2002

FIG. 1A-1

0.6. FIG.	CLASS (SUBCLASS		
APPROVED	'n	DRAFISMAN	

				_					
ATOM	57	N	ILE	9	56.124	41.944	1.328	1.00 19.03	CPS1
MOTA	58	CA	ILE	9	56.051	40.795	0.444	1.00 19.29	CPS1
MOTA	59	CB	ILE	9	55.393	39.567	1.093	1.00 21.16	CPS1
ATOM	60	CG2	ILE	9	55.354	38.416	0.080	1.00 20.76	CPS1
ATOM	61	CG1	ILE	9	56.198	39.115	2.308	1.00 19.57	CPS1
ATOM	62	CD1		9	55.5 6 0	37.946	3.081	1.00 21.48	CPS1
ATOM	63	C	ILE	9	55.161	41.304	-0.683		
ATOM	64	ō	ILE	9	54.102			1.00 20.60	CPS1
						41.904	-0.431	1.00 18.57	CPS1
ATOM	65	N	THR	10	55.601	41.100	-1.916	1.00 20.85	CPS1
ATOM	6 6	CA	THR	10	54.828	41.556	-3.064	1.00 22.77	CPS1
MOTA	67	CB	THR	10	55.555	42.710	-3.789	1.00 25.32	CPS1
MOTA	68	OG1	THR	10	55.699	43.816	-2.889	1.00 26.50	CPS1
ATOM	69	CG2	THR	10	54.758	43.168	-5.014	1.00 26.33	CPS1
ATOM	70	C	THR	10	54.598	40.400	-4.028	1.00 22.74	CPS1
ATOM	71	0	THR	10	55.506	39.633	-4.314	1.00 21.67	CPS1
ATOM	72	N	GLU	11	53.359	40.270	-4.495	1.00 24.96	CPS1
ATOM	73	CA	GLU	11	52.993	39.223	-5.445	1.00 25.76	CPS1
ATOM	74	CB	GLU	11	51.475	38.995	-5.394	1.00 28.49	
ATOM	75	CG	GLU	11	50.969	37.968			CPS1
ATOM	76	CD					-6.383	1.00 31.23	CPS1
			GLU	11	49.445	37.895	-6.440	1.00 34.90	CPS1
ATOM	77		GLU	11	48.773	38.865	-6.019	1.00 33.91	CPS1
ATOM	78	OE2		11	48.923	36.867	-6.92 6	1.00 35.55	CPS1
ATOM	79	C	GLU	11	53.420	39.693	-6.842	1.00 25.44	CPS1
MOTA	80	0	GLU	11	53.000	40.761	-7.293	1.00 24.85	CPS1
MOTA	81	N	LEU	12	54.252	38.912	-7.525	1.00 26.00	CPS1
MOTA	82	CA	LEU	12	54.715	39.316	-8.857	1.00 27.71	CPS1
ATOM	83	CB	LEU	12	55.599	38.242	-9.488	1.00 28.64	CPS1
ATOM	84	CG	LEU	12	56.860	37.729	-8.793	1.00 31.06	CPS1
ATOM	85		LEU	12	57.721	37.022	-9.836	1.00 31.75	CPS1
ATOM	86		LEU	12	57.643	38.862	-8.157	1.00 31.73	CPS1
ATOM	87	C	LEU	12	53.557	39.608		1.00 31.13	CPS1
ATOM	88		LEU				-9.810		
		0		12	53.630		-10.631	1.00 28.32	CPS1
ATOM	89	N	ALA	13	52.498	38.813	-9.708	1.00 29.63	CPS1
ATOM	90	CA	ALA	13	51.330		-10.565	1.00 32.09	CPS1
ATOM	91	CB	ALA	13	50.281		-10.238	1.00 32.02	CPS1
ATOM	92	C	ALA	13	50.732	40.379	-10.397	1.00 33.63	CPS1
ATOM	93	0	ALA	13	50.280	41.000	-11.369	1.00 33.79	CPS1
ATOM	94	N	ARG	14	50.732	40.864	-9.160	1.00 34.46	CPS1
ATOM	95	CA	ARG	14	50.188	42.178	-8.846	1.00 35.63	CPS1
ATOM	96	CB	ARG	14	50.170	42.380	-7.330	1.00 38.10	CPS1
ATOM	97	CG	ARG	14	48.818	42.770	-6.772	1.00 41.02	CPS1
ATOM	98	CD	ARG	14	48.815	44.197	-6.276	1.00 42.88	CPS1
ATOM	99	NE	ARG	14	49.762	44.395	-5.183	1.00 43.99	CPS1
ATOM	100	CZ	ARG	14	50.030	45.575	-4.628	1.00 45.35	CPS1
ATOM	101	NH1							
				14	49.420	46.670	-5.063	1.00 46.27	CPS1
ATOM	102		ARG	14	50.915	45.664	-3.642	1.00 44.46	CPS1
ATOM	103	С	ARG	14	51.022	43.264	-9.508	1.00 36.31	CPS1
ATOM	104	0	ARG	14	50.484	44.232	-10.055	1.00 36.04	CPS1
ATOM	105	N	ILE	15	52.340	43.095	-9.457	1.00 35.62	CPS1
ATOM	106	CA	ILE	15	53.258	44.046	-10.062	1.00 36.49	CPS1
ATOM	107	CB	ILE	15	54.720	43.639	-9.788	1.00 34.84	CPS1
ATOM	108		ILE	15	55.666		-10.646	1.00 34.69	CPS1
ATOM	109		ILE	15	55.037	43.835	-8.298	1.00 32.18	CPS1
ATOM	110		ILE	15	54.936	45.275	-7.834	1.00 32.10	CPS1
ATOM	111	CDI	ILE	15	52.995		-11.566	1.00 33.49	CPS1
									CPS1
ATOM	112	0	ILE	15	53.103		-12.195	1.00 38.89	
ATOM	113	N	ALA	16	52.651	42.946	-12.141	1.00 41.54	CPS1



SEP 0 9 2002

FIG. 1A-2

16.	SUBCLASS	
0.6.5	CLASS	
AFFROVED	≻	DRAFTSMAH

ATOM	114	CA	ALA	16	52.336	42.887 -13.564	1.00 44.64	CPS1
ATOM	115	CB	ALA	16	52.211	41.436 -14.018	1.00 44.42	CPS1
ATOM	116	С	ALA	16	51.016	43.629 -13.784	1.00 46.09	CPS1
ATOM	117	0	ALA	16	50.869	44.377 -14.746	1.00 47.05	CPS1
ATOM	118	N	SER	17	50.064	43.425 -12.877	1.00 49.05	CPS1
MOTA	119	CA	SER	17	48.752	44.076 -12.959	1.00 51.73	CPS1
ATOM	120	CB	SER	17	47.823	43.567 -11.851	1.00 51.91	CPS1
ATOM	121	OG	SER	17	47.472	42.208 -12.048	1.00 53.45	CPS1
ATOM	122	С	SER	17	48.851	45.594 -12.854	1.00 53.68	CPS1
ATOM	123	0	SER	17	48.310	46.316 -13.691	1.00 54.03	
ATOM	124	N	MET	18	49.530	46.075 -11.816	1.00 55.71	CPS1
ATOM	125	CA	MET	18	49.697	47.511 -11.611	1.00 57.69	CPS1
ATOM	126	CB	MET	18	50.429	47.787 -10.293	1.00 57.69	CPS1
ATOM	127	CG	MET	18	49.679	47.357 -9.046	1.00 60.86	CPS1
ATOM	128	SD	MET	18	50.678	47.547 -7.546	1.00 60.86	CPS1
ATOM	129	CE	MET	18	50.115	49.133 -6.944		CPS1
ATOM	130	c	MET	18	50.489	48.126 -12.758	1.00 63.23	CPS1
ATOM	131	ō	MET	18	50.147	49.200 -13.253	1.00 58.14	CPS1
ATOM	132	N	ALA	19	51.545		1.00 58.47	CPS1
ATOM	133	CA	ALA	19		47.440 -13.178	1.00 58.63	CPS1
ATOM	134	CB	ALA	19	52.393	47.930 -14.257	1.00 59.73	CPS1
ATOM	135	C	ALA	19	53.432	46.881 -14.626	1.00 58.94	CPS1
ATOM	136	0	ALA		51.593	48.320 -15.490	1.00 61.14	CPS1
ATOM	137	N	GLY	19	51.267	49.491 -15.679	1.00 61.35	CPS1
ATOM	138	CA	GLY	20	51.282	47.329 -16.322	1.00 62.81	CPS1
ATOM				20	50.537	47.568 -17.549	1.00 64.34	CPS1
ATOM	139	С	GLY	20	49.331	48.486 -17.438	1.00 65.24	CPS1
ATOM	140	0	GLY	20	49.010	49.210 -18.382	1.00 65.67	CPS1
ATOM	141	N	ARG	21	48.660	48.459 -16.292	1.00 65.86	CPS1
	142	CA	ARG	21	47.485	49.295 -16.081	1.00 66.76	CPS1
ATOM	143	CB	ARG	21	46.595	48.672 -14.996	1.00 68.01	CPS1
ATOM	144	CG	ARG	21	45.294	49.417 -14.698	1.00 70.30	CPS1
ATOM	145	CD	ARG	21	44.482	49.731 -15.959	1.00 72.22	CPS1
ATOM	146	NE	ARG	21	44.987	50.908 -16.671	1.00 73.68	CPS1
ATOM	147	cz	ARG	21	44.415	51.435 -17.750	1.00 74.14	CPS1
MOTA	148		ARG	21	43.314	50.891 -18.253	1.00 74.30	CPS1
ATOM	149	NH2	ARG	21	44.941	52.510 -18.324	1.00 74.39	CPS1
ATOM	150	С	ARG	21	47.862	50.728 -15.703	1.00 66.35	CPS1
MOTA	151	0	ARG	21	47.312	51.296 -14.759	1.00 66.83	CPS1
ATOM	152	N	GLN	22	48.803	51.304 -16.450	1.00 65.49	CPS1
ATOM	153	CA	GLN	22	49.263	52.676 -16.219	1.00 64.27	CPS1
ATOM	154	CB	GLN	22	50.068	52.755 -14.913	1.00 64.78	CPS1
ATOM	155	CG	GLN	22	49.187	52.941 -13.675	1.00 66.23	CPS1
ATOM	156	CD	GLN	22	49.924	52.717 -12.368	1.00 67.13	
ATOM	157	OE1	GLN	22	50.946	53.353 -12.097	1.00 67.13	CPS1
ATOM	158	NE2	GLN	22	49.401	51.812 -11.544	1.00 67.13	CPS1
ATOM	159	C	GLN	22	50.086	53.230 -17.393		CPS1
ATOM	160	0	GLN	22	49.559	53.962 -18.239	1.00 62.83	CPS1
ATOM	161	N	GLY	23	51.368	52.878 -17.452	1.00 63.71	CPS1
ATOM	162	CA	GLY	23	52.215		1.00 59.93	CPS1
ATOM	163	c	GLY	23	53.259	53.360 -18.532	1.00 54.65	CPS1
ATOM	164	ō	GLY	23		54.325 -18.006	1.00 51.39	CPS1
ATOM	165	N	ARG	23	53.852	55.099 -18.765	1.00 50.70	CPS1
ATOM	166	CA	ARG	24	53.474	54.268 -16.694	1.00 47.29	CPS1
ATOM	167	CB	ARG		54.433	55.121 -16.007	1.00 42.63	CPS1
ATOM	168	CG		24	53.798	56.490 -15.771	1.00 45.51	CPS1
ATOM	169	CD	ARG	24	54.684	57.512 -15.095	1.00 48.36	CPS1
ATOM	170		ARG	24	54.194	58.925 -15.397	1.00 50.96	CPS1
	1/0	NE	ARG	24	52.773	59.092 -15.108	1.00 53.61	CPS1



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-3

APPROVED D.G. F1G.

8 Y CLASS SUBCLASS

DRAFTSMAH

ATC				24	52.092	60.215 -15.320	1.00 54.82	CPS1
ATC			1 ARG	24	52.704	61.281 -15.824	1.00 55.59	CPS1
ATC			2 ARG	24	50.796	60.270 -15.039	1.00 55.48	CPS1
ATC			ARG	24	54.842	54.480 -14.673	1.00 38.31	CPS1
ATC			ARG	24	55.617	55.045 -13.906	1.00 35.06	CPS1
ATC			PHE	25	54.338	53.279 -14.420	1.00 34.51	CPS1
ATC			PHE	25	54.630	52.585 -13.166	1.00 32.21	CPS1
ATO			PHE	25	53.805	51.298 -13.074	1.00 33.02	CPS1
ATO			PHE	25	54.016	50.536 -11.797	1.00 33.13	CPS1
ATO			1 PHE	25	54.917	49.482 -11.741	1.00 33.65	CPS1
ATO			2 PHE	25	53.323	50.889 -10.642	1.00 34.84	CPS1
ATO			1 PHE	25	55.129	48.784 -10.553	1.00 33.64	CPS1
ATO			2 PHE	25	53.527	50.201 -9.450	1.00 34.46	CPS1
ATO			PHE	25	54.432	49.146 -9.405	1.00 34.16	CPS1
ATO			PHE	25	56.103	52.273 -12.902	1.00 29.41	CPS1
ATO			PHE	25	56.632	52.657 -11.862	1.00 29.18	CPS1
ATO			ALA	26	56.771	51.585 -13.826	1.00 26.94	CPS1
ATO			ALA	26	58.177	51.245 -13.621	1.00 25.77	CPS1
ATO			ALA	26	58.702	50.403 -14.785	1.00 25.23	CPS1
ATO			ALA	26	59.043	52.480 -13.459	1.00 25.39	CPS1
ATO			ALA	26	59.955	52.511 -12.632	1.00 22.61	CPS1
ATO			GLU	27	58.757	53.502 -14.260	1.00 24.05	CPS1
ATO			GLU	27	59.537	54.726 -14.210	1.00 25.73	CPS1
ATO			GLU	27	59.225	55.589 -15.436	1.00 25.99	CPS1
ATO			GLU	27	59.695	54.987 -16.750	1.00 26.79	CPS1
ATO			GLU	27	58.896	53.770 -17.202	1.00 28.20	CPS1
ATO			GLU	27	57.680	53.695 -16.908	1.00 30.98	CPS1
ATO			GLU	27	59.481	52.894 -17.877	1.00 29.45	CPS1
ATO			GLU	27	59.315	55.519 -12.924	1.00 26.62	CPS1
ATO			GLU	27	60.158	56.322 -12.532	1.00 27.44	CPS1
ATO			ARG	28	58.179	55.312 -12.272	1.00 26.83	CPS1
ATO			ARG	28	57.924	56.002 -11.014	1.00 28.43	CPS1
ATO			ARG	28	56.422	56.062 -10.727	1.00 31.75	CPS1
ATO			ARG	28	55.736	57.322 -11.243	1.00 38.22	CPS1
ATO			ARG	28	54.229	57.195 -11.093	1.00 41.94	CPS1
ATON			ARG	28	53.891	56.446 -9.885	1.00 46.44	CPS1
ATON			ARG	28	53.088	55.387 -9.869	1.00 47.55	CPS1
ATON			ARG	28	52.534	54.953 -11.000	1.00 48.25	CPS1
ATON			ARG	28	52.855	54.751 -8.726	1.00 49.13	CPS1
ATON			ARG	28	58.629	55.267 -9.877	1.00 27.14	CPS1
ATON			ARG	28	59.086	55.885 -8.928	1.00 27.28	CPS1
ATON			ILE	29	58.729	53.944 -9.985	1.00 26.44	CPS1
ATON			ILE	29	59.363	53.137 -8.938	1.00 26.04	CPS1
ATON			ILE	29	58.901	51.657 -9.004	1.00 26.47	CPS1
ATOM			ILE	29	59.520	50.865 -7.858	1.00 28.14	CPS1
ATOM			ILE	29	57.374	51.565 -8.976	1.00 27.67	CPS1
ATOM			ILE	29	56.722	52.214 -7.796	1.00 28.72	CPS1
ATON			ILE	29	60.888	53.122 -8.980	1.00 25.23	CPS1
ATOM			ILE	29	61.549	53.123 -7.934	1.00 25.57	CPS1
ATOM			LEU	30	61.445	53.119 -10.188	1.00 23.44	CPS1
ATOM			LEU	30	62.885	53.031 -10.371	1.00 22.74	CPS1
ATOM			LEU	30	63.185	52.029 -11.487	1.00 22.73	CPS1
ATOM			LEU	30	62.509	50.656 -11.381	1.00 22.89	CPS1
ATOM			LEU	30	62.817	49.861 -12.635	1.00 22.68	CPS1
ATOM			LEU	30	63.004	49.922 -10.126	1.00 22.78	CPS1
ATOM			LEU	30	63.590	54.344 -10.686	1.00 23.94	CPS1
ATOM	227	0	LEU	30	63.027	55.228 -11.336	1.00 23.90	CPS1
						550		



ATOM

228 N THR 31

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SEP 0 9 2002

FIG. 1A-4

64.830 54.451 -10.224

TECH CENTER 1600/2900

1.00 24.75

CPS1



ATOM 229 CA THR 31 65.643 55.636 -10.461 1.00 25.03 CPS1 ATOM 230 CB THR 31 66.787 55.749 -9.457 1.00 26.35 CPS1 ATOM 231 OG1 THR 31 67.725 54.692 -9.695 1.00 26.00 CPS1 ATOM 232 CG2 THR 31 66.261 55.671 -8.031 1.00 26.75 CPS1 ATOM 233 С THR 31 66.271 55.469 -11.832 1.00 24.44 CPS1 ATOM 234 0 THR 31 66.163 54.416 -12.441 1.00 22.68 CPS1 ATOM 235 N ARG 32 66.963 56.503 -12.293 1.00 25.91 ATOM 236 CA ARG 32 67.607 56.458 -13.603 1.00 26.68 CPS1 ATOM 237 CB ARG 32 68,342 57,780 -13,848 1.00 26.75 CPS1 ATOM 238 CG ARG 32 68.970 57.939 -15.236 1.00 29.21 ATOM 239 CD ARG 32 69.551 59.348 -15.344 1.00 29.81 CPS1 ATOM 240 NE ARG 32 59.707 -16.684 70.015 1.00 32.75 CPS1 ATOM 241 CZ ARG 32 71.129 59.256 -17.254 1.00 34.02 CPS1 ATOM 242 NH1 ARG 32 71.916 58.404 -16.606 1.00 33.55 CPS1 ATOM 243 NH2 ARG 32 71.476 59.692 -18.464 1.00 31.94 CPS1 ATOM 244 C ARG 32 68.572 55.276 -13.728 1.00 26.02 CPS1 ATOM 245 0 ARG 32 68.539 54.542 -14.721 1.00 25.46 CPS1 ATOM 246 N SER 33 69.422 55.088 -12.721 1.00 26.77 CPS1 ATOM 247 CA SER 33 70.390 53.990 -12.725 1.00 28.08 CPS1 ATOM 248 CB SER 22 71.277 54.037 -11.473 1.00 31.22 CPS1 ATOM 249 OG SER 33 72.112 55.182 -11.481 1.00 38.13 CPS1 ATOM 250 С SER 33 69.686 52.645 -12.772 1.00 27.50 CPS1 ATOM 251 0 SER 33 70.113 51.738 -13.487 1.00 28.27 CPS1 ATOM 252 N GLU 34 68.613 52.510 -11.998 1.00 25.55 CPS1 ATOM 253 CA GLU 34 67.857 51.262 -11.970 1.00 25.24 CPS1 ATOM 254 CB GLU 34 66.842 51.298 -10.822 1.00 25:04 CPS1 ATOM 255 CG GLU 34 67.531 51.247 -9.455 1.00 24.32 CPS1 ATOM 256 CD GLU 34 66.575 51.424 -8.280 1.00 26.32 CPS1 ATOM 257 OE1 GLU 34 66.860 50.849 -7.202 1.00 24.86 CPS1 ATOM OE2 GLU 258 34 65.557 52.145 -8.423 1.00 25.42 CPS1 ATOM 259 С GLU 34 67,167 50.997 -13.302 1.00 25.57 CPS1 ATOM 260 0 GLU 34 67.113 49.852 -13.767 1.00 26.12 CPS1 ATOM 261 N LEU 35 66.649 52.056 -13.919 1.00 25.65 CPS1 ATOM 262 CA LEU 35 65.978 51.931 -15.209 1.00 25.43 CPS1 ATOM 263 CB LEU 35 65.362 53.269 -15.626 1.00 24.81 CPS1 ATOM 264 CG LEU 35 64.044 53.625 -14.936 1.00 25.80 CPS1 ATOM 265 CD1 LEU 35 63.598 55.028 -15.354 1.00 24.72 CPS1 ATOM 266 CD2 LEU 35 62.980 52.592 -15.320 1.00 24.55 CPS1 ATOM 267 С LEU 35 66.961 51.465 -16.278 1.00 25.60 CPS1 ATOM 268 0 LEH 35 66.608 50.663 -17.139 1.00 25.96 CPS1 ATOM 269 N ASP 36 68.189 51.968 -16.213 1.00 26.39 CPS 1 ATOM 270 CA ASP 36 69.221 51.586 -17.176 1.00 28.65 CPS1 ATOM 271 СВ ASP 36 70.549 52,267 -16,814 1.00 30.67 CPS1 ATOM 272 CG ASP 36 71.653 51.992 -17.834 1.00 34.97 CPS1 ATOM 273 OD1 ASP 36 71.397 52.122 -19.045 1.00 36.35 CPS1 ATOM 274 OD2 ASP 36 72.780 51.653 -17.421 1.00 38.35 CPS1 ATOM 275 c ASP 36 69.374 50.061 -17.176 1.00 29.59 CPS1 ATOM 276 0 ASP 36 69.510 49.429 -18.229 1.00 29.62 CPS1 ATOM 277 N GLN 37 69.331 49.466 -15.987 1.00 29.16 CPS1 ATOM CA 278 GLN 37 69.446 48.019 -15.860 1.00 27.84 CPS1 ATOM 279 CR GLN 37 69.737 47.648 -14.404 1.00 29.01 CPS1 ATOM 280 CG GLN 37 70.983 48.305 -13.850 1.00 32.00 CPS1 ATOM 281 CD GLN 37 71.075 48.186 -12.348 1.00 34.39 CPS1 ATOM 282 OE1 GLN 37 71.087 47.079 -11.805 1.00 34.90 CPS1 ATOM 283 NE2 GLN 37 71.142 49.329 -11.662 1.00 34.48 CPS1 ATOM 284 С GLN 37 68.156 47.335 -16.301 1.00 27.75 CPS1



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-5

APPROVED O G. FIG.

EY CLASS SUBCLASS
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The second second									
ATOM	285	0	GLN	37	68.183	46.328	-17.012	1.00 27.75	ana.
ATOM	286	N	TYR	38	67.031		-15.858	1.00 26.28	CPS1
ATOM	287	CA	TYR	38	65.705		-16.167	1.00 25.28	CPS1 CPS1
ATOM	288	CB	TYR	38	64.657		-15.500	1.00 25.99	
ATOM	289	CG	TYR	38	63.213		-15.772	1.00 26.20	CPS1
ATOM	290	CD:	1 TYR	38	62.468		-16.688	1.00 26.20	CPS1
ATOM	291	CE:	1 TYR	38	61.121		-16.903	1.00 26.19	CPS1
ATOM	292	CD:	2 TYR	38	62.567		-15.074	1.00 26.29	CPS1
ATOM	293	CE:	TYR	38	61.219		-15.280	1.00 25.67	CPS1
ATOM	294	CZ	TYR	38	60.501		-16.200	1.00 28.03	CPS1
ATOM	295	OH	TYR	38	59.166		-16.428	1.00 27.03	CPS1 CPS1
ATOM	296	С	TYR	38	65.420		-17.668	1.00 26.52	CPS1
ATOM	297	0	TYR	38	64.912		-18.122	1.00 23.95	CPS1
ATOM	298	N	TYR	39	65.756		-18.440	1.00 26.98	CPS1
ATOM	299	CA	TYR	39	65.502		-19.880	1.00 20.38	CPS1
ATOM	300	CB	TYR	39	65.757		-20.488	1.00 28.06	CPS1
ATOM	301	CG	TYR	39	64.725		-20.060	1.00 27.09	CPS1
ATOM	302	CDI	TYR	39	63.365		-20.080	1.00 26.88	CPS1
ATOM	303	CEI	TYR	39	62.402		-19.691	1.00 26.96	CPS1
ATOM	304	CD2	TYR	39	65.109		-19.641	1.00 26.42	CPS1
ATOM	305	CE2	TYR	39	64.154		-19.245	1.00 27.05	CPS1
ATOM	306	CZ	TYR	39	62.806		-19.274	1.00 26.67	CPS1
ATOM	307	OH	TYR	39	61.856		-18.876	1.00 27.91	CPS1
ATOM	308	С	TYR	39	66.279		-20.641	1.00 31.26	CPS1
ATOM	309	0	TYR	39	65.899		-21.750	1.00 32.43	CPS1
ATOM	310	N	GLU	40	67.351		-20.046	1.00 32.52	CPS1
ATOM	311	CA	GLU	40	68.150		-20.690	1.00 33.92	CPS1
ATOM	312	CB	GLU	40	69.602		-20.207	1.00 35.68	CPS1
ATOM	313	CG	GLU	40	70.340		-20.579	1.00 38.76	CPS1
ATOM	314	CD	GLU	40	70.370		-22.079	1.00 41.13	CPS1
ATOM	315		GLU	40	70.557		-22.835	1.00 43.88	CPS1
ATOM	316	OE2	GLU	40	70.220		-22.501	1.00 41.69	CPS1
ATOM	317	С	GLU	40	67.616		-20.419	1.00 34.35	CPS1
ATOM	318	0	GLU	40	68.089	43.177	-21.008	1.00 33.76	CPS1
ATOM	319	N	LEU	41	66.626	44.036	-19.541	1.00 33.60	CPS1
ATOM	320	CA	LEU	41	66.080	42.733	-19.176	1.00 34.81	CPS1
ATOM	321	CB	LEU	41	65.658		-17.702	1.00 33.78	CPS1
ATOM	322	CG	LEU	41	66.725	43.183	-16.690	1.00 33.47	CPS1
ATOM	323		LEU	41	66.084	43.291	-15.309	1.00 33.49	CPS1
ATOM	324		LEU	41	67.879	42.188	-16.678	1.00 33.26	CPS1
ATOM	325	С	LEU	41	64.910	42.221	-20.013	1.00 35.00	CPS1
ATOM	326	0	LEU	41	64.199		-20.654	1.00 34.86	CPS1
ATOM	327	N	SER	42	64.713	40.904	-19.984	1.00 36.21	CPS1
ATOM ATOM	328	CA	SER	42	63.615	40.271	-20.709	1.00 37.02	CPS1
ATOM	329	CB	SER	42	63.788	38.752	-20.716	1.00 37.19	CPS1
ATOM	330	OG	SER	42	63.601		-19.413	1.00 37.95	CPS1
ATOM	331	С	SER	42	62.321		-19.986	1.00 37.67	CPS1
ATOM	332	0	SER	42	62.355	41.124	-18.856	1.00 37.09	CPS1
ATOM	333	N	GLU	43	61.180	40.378	-20.618	1.00 37.74	CPS1
ATOM	334	CA	GLU	43	59.917		-19.970	1.00 39.67	CPS1
	335	CB	GLU	43	58.716	40.282	-20.829	1.00 42.30	CPS1
ATOM ATOM	336	CG	GLU	43	57.421		-20.417	1.00 46.74	CPS1
ATOM	337	CD	GLU	43	56.177		-21.122	1.00 49.57	CPS1
ATOM	338		GLU	43	56.253		-22.333	1.00 51.74	CPS1
ATOM	339		GLU	43	55.116		-20.465	1.00 50.82	CPS1
ATOM	340 341	C	GLU	43	59.833		-18.611	1.00 38.42	CPS1
	341	J	GLU	43	59.425	40.619	-17.623	1.00 37.06	CPS1



SEP 0 9 2002

FIG. 1A-6



MOTA	342	N	LYS	44	60.223	38.743 -18.567	1.00 37.89	CPS1
ATOM	343	CA	LYS	44	60.176	37.985 -17.318	1.00 38.86	CPS1
ATOM	344	CB	LYS	44	60.566	36.525 -17.562	1.00 40.32	CPS1
ATOM	345	CG	LYS	44	60.777	35.706 -16.292	1.00 43.45	CPS1
ATOM	346	CD	LYS	44	60.766	34.214 -16.594	1.00 46.17	CPS1
MOTA	347	CE	LYS	44	61.613	33.425 -15.603	1.00 47.94	CPS1
ATOM	348	NZ	LYS	44	63.073	33.691 -15.805	1.00 50.56	CPS1
ATOM	349	C	LYS	44	61.086	38.587 -16.257	1.00 37.33	CPS1
ATOM	350	0	LYS	44	60.661	38.823 -15.127	1.00 36.33	CPS1
ATOM	351	N	ARG	45	62.338	38.835 -16.625	1.00 36.56	CPS1
ATOM	352	CA	ARG	45	63.310	39.403 -15.695	1.00 35.88	CPS1
ATOM	353	CB	ARG	45	64.700	39.412 -16.333	1.00 37.23	CPS1
ATOM	354	CG	ARG	45	65.356	38.041 -16.385		
							1.00 39.66	CPS1
ATOM	355	CD	ARG	45	65.840	37.633 -15.008	1.00 42.70	CPS1
ATOM	356	NE	ARG	45	66.842	38.569 -14.498	1.00 45.11	CPS1
MOTA	357	CZ	ARG	45	66.700	39.307 -13.399	1.00 46.10	CPS1
ATOM	358	NH1	ARG	45	65.593	39.226 -12.672	1.00 45.56	CPS1
ATOM	359	NH2	ARG	45	67.666	40.140 -13.033	1.00 47.39	CPS1
ATOM	360	С	ARG	45	62.920	40.807 -15.254	1.00 34.51	CPS1
ATOM	361	ō	ARG	45	63.182	41.200 -14.120		
							1.00 33.99	CPS1
ATOM	362	N	LYS	46	62.294	41.565 -16.148	1.00 32.94	CPS1
MOTA	363	CA	LYS	46	61.857	42.911 -15.802	1.00 32.28	CPS1
ATOM	364	CB	LYS	46	61.165	43.580 -16.990	1.00 32.34	CPS1
MOTA	365	CG	LYS	46	62.109	44.110 -18.051	1.00 32.52	CPS1
ATOM	366	CD	LYS	46	61.327	44.905 -19.113	1.00 33.61	CPS1
ATOM	367	CE	LYS	46	62.262	45.515 -20.151	1.00 34.98	CPS1
ATOM	368	NZ	LYS	46	61.505	46.250 -21.211	1.00 36.94	CPS1
ATOM	369	C	LYS	46				
					60.888	42.868 -14.621	1.00 31.45	CPS1
ATOM	370	0	LYS	46	61.002	43.655 -13.684	1.00 30.01	CPS1
MOTA	371	N	ASN	47	59.937	41.942 -14.672	1.00 30.18	CPS1
ATOM	372	CA	ASN	47	58.951	41.806 -13.606	1.00 30.39	CPS1
ATOM	373	CB	ASN	47	57.886	40.773 -14.012	1.00 32.50	CPS1
ATOM	374	CG	ASN	47	56.914	40.449 -12.885	1.00 35.59	CPS1
ATOM	375	OD1	ASN	47	57.020	39.401 -12.246	1.00 39.44	CPS1
ATOM	376		ASN	47	55.969	41.346 -12.635	1.00 35.35	CPS1
ATOM	377	C	ASN	47	59.608			
ATOM						41.424 -12.273	1.00 28.81	CPS1
	378	0	ASN	47	59.252	41.971 -11.230	1.00 27.56	CPS1
ATOM	379	N	GLU	48	60.568	40.503 -12.308	1.00 27.77	CPS1
ATOM	380	CA	GLU	48	61.265	40.064 -11.093	1.00 26.38	CPS1
ATOM	381	CB	GLU	48	62.172	38.870 -11.417	1.00 30.74	CPS1
ATOM	382	CG	GLU	48	61.417	37.675 -12.004	1.00 34.10	CPS1
ATOM	383	CD	GLU	48	62.338	36.589 -12.553	1.00 37.43	CPS1
ATOM	384		GLU	4.8	61.815	35.595 -13.106	1.00 38.39	CPS1
ATOM	385		GLU	48	63.577	36.727 -12.434	1.00 38.18	CPS1
ATOM	386	C	GLU					
ATOM				48	62.101	41.201 -10.498	1.00 26.11	CPS1
	387	0	GLU	48	62.132	41.416 -9.271	1.00 22.48	CPS1
ATOM	388	N	PHE	49	62.792	41.919 -11.377	1.00 23.64	CPS1
ATOM	389	CA	PHE	49	63.628	43.042 -10.976	1.00 24.48	CPS1
ATOM	390	CB	PHE	49	64.356	43.591 -12.197	1.00 24.05	CPS1
ATOM	391	CG	PHE	49	65.252	44.754 -11.903	1.00 24.66	CPS1
ATOM	392		PHE	49	66.591	44.552 -11.572	1.00 26.69	CPS1
MOTA	393		PHE	49	64.771			
ATOM	394		PHE			46.052 -11.982	1.00 23.63	CPS1
				49	67.438	45.632 -11.329	1.00 27.13	CPS1
ATOM	395		PHE	49	65.601	47.137 -11.743	1.00 25.03	CPS1
ATOM	396	CZ	PHE	49	66.938	46.933 -11.416	1.00 26.71	CPS1
ATOM	397	C	PHE	49	62.777	44.152 -10.364	1.00 23.89	CPS1
ATOM	398	0	PHE	49	63.124	44.721 -9.323	1.00 24.30	CPS1
				-				



SEP 0 9 2002 **TECH CENTER 1600/2900**

FIG. 1A-7

SS	ATOM	399	N	LEU	50
15	ATOM	400	CA	LEU	50
Sueci.	ATOM	401	CB	LEU	50
7 3	ATOM	402	CG	LEU	50
. 60	ATOM	403	CDI		50
LASS	ATOM	404	CD2		50
ದ!ಕ	ATOM	405	C	LEU	50
o **	ATOM	406	ō	LEU	50
¥ . ¥	ATOM	407	N	ALA	51
1 2 1	ATOM	408	CA	ALA	51
A A	ATOM	409	CB	ALA	51
-	ATOM	410	c	ALA	51
	ATOM	411	ō	ALA	51
	ATOM	412	N	GLY	52
	ATOM	413	CA	GLY	52
	ATOM	414	C	GLY	52
	ATOM	415	ō	GLY	52
	ATOM	416	N	ARG	53
	ATOM	417	CA	ARG	53
	ATOM	418	CB	ARG	
	ATOM	419	CG	ARG	53
	ATOM	420	CD	ARG	53
	ATOM	421	NE	ARG	53
	ATOM	422	CZ	ARG	53
	ATOM	423	NH1	ARG	53
	ATOM	424	NH2	ARG	53
	ATOM	425	C	ARG	53
	ATOM	426	0	ARG	53
	ATOM	427	N	PHE	53
	ATOM	428	CA	PHE	54
	ATOM	429	CB	PHE	54
	ATOM	430	CG	PHE	54
	ATOM	431	CD1	PHE	54
	ATOM	432	CD2	PHE	54
	ATOM	433	CE1	PHE	54
	ATOM	434	CE2	PHE	54 54
	ATOM	435	CZ	PHE	
	ATOM	436	C	PHE	54
	ATOM	437	0	PHE	54 54
	ATOM	438	N	ALA	
	ATOM	439	CA	ALA	55
	ATOM	440	CB	ALA	55
	ATOM	441	C	ALA	55
	ATOM	442	0	ALA	55
	ATOM	443	N	ALA	55
	ATOM	444	CA	ALA	56
	ATOM	445	CB	ALA	56
	ATOM	446	CB	ALA	56
	ATOM	447	0		56
	ATOM	448	и	ALA	56
	ATOM	448	CA	LYS	57
	ATOM	449		LYS	57
	ATOM	450	CB	LYS	57
	ATOM	451	CG	LYS	57

ATOM

ATOM

ATOM

ATOM

LYS

LYS

LYS

452 CD

454 NZ

455 C

453 CE LYS 57

57

57

57

11G. 1A-/				
61.672	44.476	-11.029	1.00 22.90	CPS1
60.795	45.534	-10.557	1.00 23.71	CPS1
59.732	45.836	-11.617	1.00 24.35	CPS1
58.714	46.928	-11.325	1.00 25.33	CPS1
59.403	48.253	-11.010	1.00 24.88	CPS1
57.805	47.055	-12.536	1.00 25.38	CPS1
60.132	45.138	-9.236	1.00 23.44	CPS1
60.011	45.957	-8.322	1.00 22.54	
59.698	43.884	-9.148	1.00 22.99	CPS1
59.056	43.399	-7.929	1.00 23.20	CPS1
58.581	41.959	-8.123		CPS1
60.034	43.476	-6.754		CPS1
59.655	43.884	-5.653		CPS1
61.284	43.089	-6.998		CPS1
62.297	43.120	-5.951	1.00 21.48	CPS1
62.585	44.523	-5.460	1.00 22.37	CPS1
62.715			1.00 22.17	CPS1
62.675	44.764 45.461	-4.256	1.00 21.91	CPS1
		-6.402	1.00 23.24	CPS1
62.933	46.862	-6.076	1.00 23.63	CPS1
63.169	47:654	-7.364	1.00 25.69	CPS1
64.546	48.242	-7.490	1.00 29.63	CPS1
65.618	47.212	-7.338	1.00 28.33	CPS1
66.937	47.751	-7.675	1.00 29.58	CPS1
67.976	46.986	-7.980	1.00 29.37	CPS1
67.821	45.670	-7.978	1.00 29.23	CPS1
69.153	47.525	-8.299	1.00 26.48	CPS1
61.752	47.468	-5.336	1.00 23.34	CPS1
61.921	48.237	-4.389	1.00 22.79	CPS1
60.551	47.146	-5.801	1.00 22.67	CPS1
59.335	47.638	-5.181	1.00 22.96	CPS1
58.114	47.106	-5.947	1.00 22.72	CPS1
56.807	47.619	-5.429	1.00 24.49	CPS1
56.074	46.882	-4.506	1.00 24.85	CPS1
56.329	48.865	-5.828	1.00 24.29	CPS1
54.883	47.376	-3.983	1.00 25.96	CPS1
55.143	49.370	-5.316	1.00 25.86	CPS1
54.414	48.624	-4.387	1.00 26.67	CPS1
59.285	47.177	-3.724	1.00 22.66	CPS1
59.018	47.970	-2.808	1.00 21.27	
59.556	45.896	-3.508	1.00 20.95	CPS1
59.524	45.349	-2.147	1.00 20.91	CPS1
59.733	43.846	-2.191	1.00 20.44	CPS1
60.568	45.990	-1.234		CPS1
60.288	46.295	-0.075		CPS1
61.779	46.172	-1.751		CPS1
62.861	46.761	-0.971	1.00 18.74	CPS1
64.180			1.00 19.35	CPS1
62.543	46.698	-1.762	1.00 19.52	CPS1
62.773	48.201	-0.593	1.00 20.45	CPS1
	48.617	0.543	1.00 18.52	CPS1
62.015	48.969	-1.545	1.00 18.95	CPS1
61.677	50.352	-1.270	1.00 19.87	CPS1
61.427	51.107	-2.583	1.00 19.77	CPS1
62.707	51.225	-3.393	1.00 20.64	CPS1
62.533	52.055	-4.679	1.00 21.45	CPS1
63.801	51.995	-5.512	1.00 22.31	CPS1
63.888	53.112	-6.510	1.00 22.70	CPS1
60.487	50.461	-0 320	1 00 10 05	anai

50.461 -0.329 1.00 19.95

CPS1



SEP 0 9 2002

TECH CENTER 1600/2900

FIG. 1A-8

APFROVED O.G. FIG.
SY OLASS SUBCLASS

ATOM	456	0	LYS	57	60.458	51.352	0.515	1.00 20.79	CPS1
ATOM	457	N	GLU	58	59.513	49.561	-0.463	1.00 19.28	CPS1
ATOM	458	CA	GLU	58	58.358	49.567	0.436	1.00 21.04	CPS1
ATOM	459	CB	GLU	58	57.324	48.516	0.013	1.00 22.82	CPS1
ATOM	460	CG	GLU	58	56.428	48.907	-1.170	1.00 28.45	CPS1
ATOM	461	CD	GLU	58	55.586	50.145	-0.886	1.00 31.31	CPS1
ATOM	462		GLU	58	55.244	50.371	0.295	1.00 33.36	CPS1
ATOM	463	OE2		58	55.253	50.886	-1.840	1.00 34.15	CPS1
ATOM ATOM	464 465	C O	GLU	58	58.851	49.242	1.856	1.00 19.94	CPS1
ATOM	466	N	ALA	58	58.456	49.899	2.818	1.00 19.84	CPS1
ATOM	467	CA	ALA	59 59	59.717 60.251	48.234	1.979	1.00 18.95	CPS1
ATOM	468	CB	ALA	59	61.155	47.861	3.300	1.00 19.85	CPS1
ATOM	469	C	ALA	59	61.133	49.037	3.185	1.00 18.19	CPS1
ATOM	470	Ö	ALA	59	60.954	49.359	5.076	1.00 20.46	CPS1
ATOM	471	N	PHE	60	61.831	49.691	3.042	1.00 20.70 1.00 19.23	CPS1
ATOM	472	CA	PHE	60	62.606	50.824	3.538	1.00 19.23 1.00 19.91	CPS1
ATOM	473	CB	PHE	60	63.500	51.407	2.440	1.00 19.91	CPS1
ATOM	474	CG	PHE	60	64.280	52.613	2.893	1.00 20.97	CPS1
ATOM	475	CD1	PHE	60	65.503	52.463	3.530	1.00 21.48	CPS1
ATOM	476		PHE	60	63.737	53.891	2.768	1.00 21.47	CPS1 CPS1
ATOM	477		PHE	60	66.183	53.576	4.053	1.00 22.10	CPS1
ATOM	478	CE2	PHE	60	64.403	55.017	3.286	1.00 23.29	CPS1
ATOM	479	CZ	PHE	60	65.628	54.852	3.930	1.00 23.90	CPS1
ATOM	480	C	PHE	60	61.673	51.919	4.047	1.00 20.74	CPS1
ATOM	481	0	PHE	60	61.916	52.515	5.098	1.00 21.03	CPS1
ATOM	482	N	SER	61	60.604	52.191	3.302	1.00 20.69	CPS1
MOTA	483	CA	SER	61	59.669	53.237	3.702	1.00 21.92	CPS1
ATOM	484	CB	SER	61	58.625	53.488	2.607	1.00 22.10	CPS1
ATOM	485	OG	SER	61	57.716	52.406	2.499	1.00 23.85	CPS1
ATOM	486	C	SER	61	58.967	52.917	5.020	1.00 22.52	CPS1
ATOM	487	0	SER	61	58.574	53.824	5.760	1.00 23.57	CPS1
ATOM	488	N	LYS	62	58.811	51.633	5.314	1.00 21.64	CPS1
ATOM	489	CA	LYS	62	58.170	51.220	6.563	1.00 22.44	CPS1
ATOM	490	CB	LYS	62	57.705	49.767	6.463	1.00 22.20	CPS1
ATOM	491	CG	LYS	62	56.539	49.575	5.483	1.00 25.33	CPS1
ATOM	492	CD	LYS	62	56.149	48.113	5.354	1.00 29.01	CPS1
ATOM	493	CE	LYS	62	54.862	47.975	4.560	1.00 32.68	CPS1
ATOM	494	NZ	LYS	62	54.355	46.585	4.526	1.00 36.07	CPS1
ATOM	495	С	LYS	62	59.155	51.392	7.719	1.00 22.39	CPS1
ATOM ATOM	496 497	0	LYS	62	58.782	51.841	8.806	1.00 21.87	CPS1
ATOM	497	N CA	ALA	63	60.413	51.040	7.479	1.00 20.82	CPS1
ATOM	498	CB	ALA	63	61.444	51.194	8.502	1.00 21.70	CPS1
ATOM	500	CB	ALA	63	62.755	50.574	8.022	1.00 22.55	CPS1
ATOM	501	0	ALA	63	61.633	52.688	8.786	1.00 23.41	CPS1
ATOM	502	N	PHE	63 64	61.886	53.092	9.928	1.00 22.35	CPS1
ATOM	503	CA	PHE	64	61.498	53.498	7.737	1.00 23.23	CPS1
ATOM	504	CB	PHE	64	61.638	54.946	7.838	1.00 25.59	CPS1
ATOM	505	CG	PHE	64	61.638	55.559	6.430	1.00 27.30	CPS1
ATOM	506	CD1		64	62.121	56.979	6.381	1.00 30.46	CPS1
ATOM	507		PHE	64	63.464 61.237	57.279	6.593	1.00 31.49	CPS1
ATOM	508	CE1		64	63.920	58.015	6.107	1.00 29.70	CPS1
ATOM	509		PHE	64	61.681	58.596 59.333	6.528	1.00 33.53	CPS1
ATOM	510	cz	PHE	64	63.021	59.333	6.039 6.249	1.00 31.57	CPS1
ATOM	511	č	PHE	64	60.477	55.504	8.667	1.00 32.65	CPS1
ATOM	512	ō	PHE	64	60.564	56.613		1.00 26.41	CPS1
-		-			00.564	30.613	9.193	1.00 27.04	CPS1



SEP 0 9 2002

FIG. 1A-9

16.	SUBCL ASS	
10.6.	CLASS	
APPROVED	ka .	DRAFTSMAR

ATOM	513	N	GLY	65	59.388	54.735	8.751	1.00 27.22	CPS1
ATOM	514	CA	GLY	65	58.229	55.102	9.554	1.00 28.06	CPS1
ATOM	515	С	GLY	65	57.135	55.940	8.923	1.00 29.26	CPS1
ATON	1 516	0	GLY	65	56.143	56.260	9.577	1.00 29.04	CPS1
ATOM	517	N	THR	66	57.299	56.279	7.650	1.00 29.45	CPS1
ATOM		CA	THR	66	56.333	57.119	6.951	1.00 30.32	CPS1
ATOM		CB	THR	66	57.033	58.351	6.391	1.00 30.19	CPS1
ATON			THR	66	57.997	57.922	5.424	1.00 31.68	CPS1
ATOM			THR	66	57.751	59.114	7.489	1.00 31.63	CPS1
ATON		C	THR	66	55.640	56.453	5.764	1.00 31.63	CPS1
ATOM		ō	THR	66	54.548	56.862	5.365	1.00 30.51	
ATOM		N	GLY	67	56.280	55.443	5.188	1.00 30.50	CPS1
ATOM		CA	GLY	67	55.713	54.809	4.011	1.00 30.12	CPS1
ATOM		c	GLY	67	56.020	55.750			CPS1
ATOM		ō	GLY	67	56.622	56.806	2.852	1.00 31.44	CPS1
ATOM		и	ILE	68			3.058	1.00 30.31	CPS1
ATOM		CA	ILE	68	55.626 55.886	55.383	1.639	1.00 31.40	CPS1
ATOM			ILE			56.239	0.486	1.00 32.28	CPSI
ATOM		CB	ILE	68	55.869	55.429	-0.844	1.00 31.80	CPS1
				68	56.083	56.375	-2.048	1.00 32.06	CPSI
ATOM			ILE	68	56.975	54.364	-0.826	1.00 29.99	CPSI
ATOM			·ILE	68	58.391	54.924	-0.821	1.00 29.70	CPSI
ATOM		C	ILE	68	54.812	57.315	0.429	1.00 33.69	CPSI
ATOM		0	ILE	68	53.623	57.028	0.556	1.00 34.51	CPS1
ATOM		N	GLY	69	55.233	58.558	0.248	1.00 35.19	CPS1
ATOM		CA	GLY	69	54.281	59.649	0.187	1.00 36.88	CPSI
ATOM		C	GLY	69	54.989	60.985	0.167	1.00 37.34	CPSI
ATOM		0	GLY	69	56.065	61.115	-0.413	1.00 37.87	CPSI
ATOM		N	ALA	70	54.394	61.977	0.821	1.00 38.19	CPSI
ATOM		CA	ALA	70	54.964	63.314	0.866	1.00 38.33	CPSI
ATOM		CB	ALA	70	54.010	64.252	1.609	1.00 39.53	CPSI
ATOM		С	ALA	70	56.352	63.383	1.493	1.00 38.24	CPSI
ATOM		0	ALA	70	57.188	64.171	1.067	1.00 39.11	CPSI
ATOM		N	GLN	71	56.612	62.547	2.494	1.00 38.21	CPS1
ATOM		CA	GLN	71	57.901	62.578	3.177	1.00 37.58	CPSI
ATOM	547	CB	GLN	71	57.704	62.177	4.642	1.00 40.14	CPS1
ATOM		CG	GLN	71	56.511	62.867	5.297	1.00 44.12	CPS1
ATOM	549	CD	GLN	71	56.276	62.410	6.724	1.00 45.82	CPSI
ATOM	550	OE1	GLN	71	57.140	62.570	7.587	1.00 46.65	CPSI
ATOM	551	NE2	GLN	71	55.101	61.838	6.980	1.00 46.84	CPSI
ATOM	552	С	GLN	71	58.997	61.706	2.557	1.00 35.81	CPS1
ATOM	553	0	GLN	71	60.175	61.854	2.885	1.00 35.04	CPS1
ATOM	554	N	LEU	72	58.619	60.805	1.662	1.00 33.50	CPS1
ATOM	555	CA	LEU	72	59.602	59.917	1.053	1.00 31.98	CPSI
ATOM		CB		72	59.899	58.762	2.010	1.00 30.93	CPS1
ATOM	557	CG	LEU	72	60.905	57.699	1.561	1.00 30.26	CPS1
ATOM			LEU	72	62.311	58.276	1.592	1.00 30.20	CPS1
ATOM			LEU	72	60.801	56.483	2.490	1.00 29.64	CPS1
ATOM		C	LEU	72	59.104	59.364	-0.269	1.00 30.33	CPS1
ATOM		ō	LEU	72	58.025	58.794		1.00 30.33	
ATOM		N	SER	73	59.907	59.526	-0.333	1.00 30.73	CPS1
ATOM		CA	SER	73	59.550	59.526	-1.315		CPS1
ATOM		CB	SER	73			-2.649	1.00 30.01	CPS1
ATOM		OG	SER	73	59.795	60.161	-3.679	1.00 30.79	CPS1
ATOM		C	SER	73	59.700	59.659	-5.007	1.00 33.48	CPS1
ATOM		0	SER		60.348	57.824	-3.070	1.00 28.08	CPS1
ATOM		N	PHE	73	61.447	57.596	-2.574	1.00 28.49	CPS1
ATOM				74	59.792	57.032	-3.985	1.00 28.86	CPS1
ATOM	569	CA	PHE	74	60.512	55.869	-4.502	1.00 28.18	CPS1



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-10

PROVED O. S. FIG.
BY CLASS SUBCLASS
FISHAN

ATOM	570	CB	PHE	74	59.712	55.173	-5.608	1.00 28.46	CPS1
ATOM	571	CG	PHE	74	58.581	54.331	-5.106	1.00 28.51	CPS1
ATOM	572	CD1	PHE	74	58.833	53.164	-4.398	1.00 29.22	CPS1
ATOM	573		PHE	74	57.264	54.695	-5.358	1.00 28.56	CPS1
ATOM	574	CE1	PHE	74	57.789	52.364	-3.951	1.00 29.35	CPS1
MOTA	575		PHE	74	56.213	53.907	-4.914	1.00 30.56	CPS1
ATOM	576	CZ	PHE	74	56.479	52.734	-4.209	1.00 28.99	CPS1
ATOM	577	С	PHE	74	61.818	56.377	-5.107	1.00 29.02	CPS1
ATOM	578	0	PHE	74	62.846	55.697	-5.076	1.00 28.52	CPS1
ATOM	579	N	GLN	75	61.776	57.586	-5.660	1.00 29.54	CPS1
ATOM	580	CA	GLN	75	62.959	58.168	-6.289	1.00 30.04	CPS1
ATOM	581	CB	GLN	75	62.555	59.395	-7.117	1.00 31.75	CPS1
ATOM	582	CG	GLN	75	61.636	59.056	-8.284	1.00 31.66	CPS1
ATOM	583	CD	GLN	75	62.300	58.137	-9.295	1.00 32.50	CPS1
ATOM	584		GLN	75	61.673	57.207	-9.816	1.00 34.26	CPS1
ATOM	585		GLN	75	63.571	58.396	-9.584	1.00 30.64	CPS1
ATOM	586	C	GLN	75	64.052	58.543	-5.294	1.00 30.56	CPS1
ATOM	587	0	GLN	75	65.205	58.768	-5.681	1.00 29.97	CPS1
ATOM ATOM	588	N	ASP	76	63.697	58.605	-4.011	1.00 30.64	CPS1
ATOM	589	CA	ASP	76	64.669	58.943	-2.972	1.00 29.57	CPS1
ATOM	590 591	CB	ASP	76	63.975	59.494	-1.718	1.00 30.95	CPS1
ATOM	592		ASP ASP	76	63.293	60.824	-1.955	1.00 32.86	CPS1
ATOM	593		ASP	76 76	63.804	61.614	-2.771	1.00 33.98	CPS1
ATOM	594	C	ASP	76	62.254	61.083	-1.313	1.00 32.57	CPS1
ATOM	595	0	ASP	76	65.472 66.430	57.720	-2.546	1.00 28.65	CPS1
ATOM	596	N	ILE	77		57.835	-1.788	1.00 28.90	CPS1
ATOM	597	CA	ILE	77	65.085 65.752	56.551 55.318	-3.038	1.00 27.41	CPS1
ATOM	598	CB	ILE	77	64.750	54.372	-2.644 -1.947	1.00 26.26	CPS1
ATOM	599		ILE	77	65.494	53.213	-1.295	1.00 25.85 1.00 26.27	CPS1
ATOM	600		ILE	77	63.927	55.145	-0.912	1.00 25.55	CPS1
ATOM	601		ILE	77	62.613	54.455	-0.547	1.00 25.71	CPS1 CPS1
ATOM	602	С	ILE	77	66.323	54.562	-3.830	1.00 26.41	CPS1
ATOM	603	0	ILE	77	65.633	54.355	-4.819	1.00 28.03	CPS1
ATOM	604	N	GLU	78	67.573	54.134	-3.726	1.00 26.24	CPS1
ATOM	605	CA	GLU	78	68.179	53.359	-4.800	1.00 26.41	CPS1
ATOM	606	CB	GLU	78	69.198	54.197	-5.586	1.00 27.49	CPS1
ATOM	607	CG	GLU	78	69.942	53.392	-6.661	1.00 31.00	CPS1
ATOM	608	CD	GLU	78	70.711	54.265	-7.657	1.00 34.35	CPS1
ATOM	609	OE1	GLU	78	70.059	54.887	-8.526	1.00 35.58	CPS1
ATOM	610	OE2	GLU	78	71.959	54.328	-7.568	1.00 34.83	CPS1
ATOM	611	С	GLU	78	68.856	52.116	-4.235	1.00 26.51	CPS1
ATOM	612	0	GLU	78	69.581	52.183	-3.244	1.00 26.47	CPS1
ATOM	613	N	ILE	79	68.595	50.976	-4.863	1.00 26.08	CPS1
ATOM	614	CA	ILE	79	69.205	49.731	-4.445	1.00 25.84	CPS1
ATOM	615	CB	ILE	79	68.192	48.545	-4.459	1.00 25.79	CPS1
MOTA	616		ILE	79	68.942	47.221	-4.467	1.00 25.99	CPS1
ATOM	617		ILE	79	67.282	48.595	-3.224	1.00 28.30	CPS1
ATOM	618		ILE	79	66.246	49.685	-3.247	1.00 25.92	CPS1
ATOM	619	C	ILE	79	70.329	49.419	-5.420	1.00 26.11	CPS1
ATOM	620	0	ILE	79	70.186	49.598	-6.633	1.00 24.92	CPS1
MOTA	621	N	ARG	80	71.455	48.974	-4.876	1.00 26.85	CPS1
ATOM	622	CA	ARG	80	72.604	48.582	-5.675	1.00 26.89	CPS1
ATOM	623	CB	ARG	80	73.708	49.616	-5.587	1.00 29.63	CPS1
ATOM	624	CG	ARG	80	73.353	50.965	-6.123	1.00 31.02	CPS1
ATOM	625	CD	ARG	80	74.524	51.844	-5.838	1.00 35.09	CPS1
MOTA	626	NE	ARG	80	74.282	53.237	-6.147	1.00 35.47	CPS1



RECEIVED SEP 0 9 2002

FIG. 1A-11

FIG.	SUBCLASS	
C.G. F	CLASS .	
APPROVES		DRAFTSMAN

7001		~~							
MOTA	627	CZ	ARG	80	75.084	54.205	-5.736	1.00 33.96	CPS1
ATOM	628		ARG	80	76.149	53.896	-5.009	1.00 32.40	CPS1
ATOM	629		ARG	80	74.824	55.460	-6.053	1.00 34.37	CPS1
ATOM	630	С	ARG	80	73.130	47.294	-5.090	1.00 27.91	CPS1
ATOM	631	0	ARG	80	72.704	46.877	-4.017	1.00 26.72	CPS1
MOTA	632	N	LYS	81	74.061	46.662	-5.794	1.00 28.40	CPS1
ATOM	633	CA	LYS	81	74.671	45.436	-5.301	1.00 29.29	
ATOM	634	CB	LYS	81	74.395	44.275	-6.260		CPS1
ATOM	635	CG	LYS	81	72.962	43.773		1.00 31.32	CPS1
ATOM	636	CD	LYS	81			-6.177	1.00 34.37	CPS1
ATOM	637	CE	LYS	81	72.745	42.490	-6.965	1.00 38.80	CPS1
ATOM					71.388	41.887	-6.623	1.00 41.39	CPS1
	638	NZ	LYS	81	71.175	40.558	-7.270	1.00 45.04	CPS1
ATOM	639	С	LYS	81	76.159	45.688	-5.173	1.00 29.85	CPS1
ATOM	640	0	LYS	81	76.754	46.332	-6.039	1.00 29.65	CPS1
MOTA	641	N	ASP	82	76.768	45.225	-4.088	1.00 28.96	CPS1
MOTA	642	CA	ASP	82	78.194	45.443	-3.952	1.00 29.85	CPS1
ATOM	643	CB	ASP	82	78.642	45.423	-2.480	1.00 29,47	CPS1
ATOM	644	CG	ASP	82	78.413	44.095	-1.796	1.00 28.92	CPS1
ATOM	645	OD1	ASP	82	78.331	43.051	-2.471	1.00 29.25	
ATOM	646	OD2	ASP	82	78.346	44.105	-0.552		CPS1
ATOM	647	С	ASP	82	78.918	44.388	-4.773	1.00 30.21	CPS1
ATOM	648	ō	ASP	82	78.281			1.00 30.66	CPS1
ATOM	649	N	GLN	83		43.626	-5.496	1.00 29.93	CPS1
ATOM	650	CA			80.239	44.342	-4.667	1.00 32.99	CPS1
ATOM			GLN	83	81.023	43.394	-5.450	1.00 34.77	CPS1
	651	CB	GLN	83	82.512	43.700	-5.287	1.00 37.08	CPS1
ATOM	652	CG	GLN	83	82.860	45.145	-5.635	1.00 38.94	CPS1
MOTA	653	CD	GLN	83	84.352	45.399	-5.653	1.00 40.99	CPS1
MOTA	654		GLN	83	85.032	45.115	-6.643	1.00 42.58	CPS1
ATOM	655	NE2	GLN	83	84.874	45.925	-4.549	1.00 41.73	CPS1
ATOM	656	С	GLN	83	80.746	41.924	-5.151	1.00 35.50	CPS1
ATOM	657	0	GLN	83	81.123	41.056	-5.930	1.00 35.54	CPS1
MOTA	658	N	ASN	84	80.094	41.640	-4.027	1.00 36.07	
ATOM	659	CA	ASN	84	79.757	40.258	-3.684		CPS1
ATOM	660	CB	ASN	84	79.863	40.014		1.00 35.57	CPS1
ATOM	661	CG	ASN	84	81.284		-2.178	1.00 37.57	CPS1
ATOM	662		ASN	84		39.960	-1.700	1.00 39.82	CPS1
ATOM	663		ASN	84	82.116	39.250	-2.270	1.00 41.25	CPS1
ATOM	664				81.577	40.702	-0.639	1.00 40.86	CPS1
ATOM		C	ASN	84	78.335	39. 93 7	-4.113	1.00 34.27	CPS1
ATOM	665	0	ASN	84	77.856	38.824	-3.899	1.00 34.98	CPS1
	666	N	GLY	85	77.659	40.914	-4.706	1.00 31.13	CPS1
ATOM	667	CA	GLY	85	76.289	40.703	-5.137	1.00 29.50	CPS1
ATOM	668	С	GLY	85	75.274	41.002	-4.040	1.00 27.83	CPS1
ATOM	669	0	GLY	85	74.089	40.743	-4.209	1.00 27.44	CPS1
MOTA	670	N	LYS	86	75.737	41.548	-2.919	1.00 26.25	CPS1
ATOM	671	CA	LYS	86	74.858	41.888	-1.797	1.00 25.96	
ATOM	672	CB	LYS	86	75.664	41.946	-0.500	1.00 26.50	CPS1
ATOM	673	CG	LYS	86	74.905	42.542			CPS1
ATOM	674	CD	LYS	86			0.680	1.00 26.15	CPS1
ATOM	675	CE	LYS	86	73.833	41.595	1.234	1.00 24.85	CPS1
ATOM	676	NZ			73.002	42.312	2.322	1.00 24.53	CPS1
ATOM	677		LYS	86	72.000	41.403	2.973	1.00 23.95	CPS1
ATOM		C	LYS	86	74.164	43.232	-2.002	1.00 24.92	CPS1
	678	0	LYS	86	74.812	44.253	-2.223	1.00 25.51	CPS1
ATOM	679	N	PRO	87	72.830	43.256	-1.938	1.00 24.79	CPS1
ATOM	680	CD	PRO	87	71.858	42.148	-1.905	1.00 26.28	CPS1
ATOM	681	CA	PRO	87	72.157	44.538	-2.123	1.00 23.90	CPS1
ATOM	682	CB	PRO	87	70.702	44.136	-2.356	1.00 25.37	CPS1
ATOM	683	CG	PRO	87	70.571	42.868	-1.581		
				÷ ·	.0.5,1	.2.008	-1.201	1.00 26.57	CPS1



SEP 0 9 2002

FIG. 1A-12



ATOM	684	C	PRO	87	72.300	45.486	-0.933	1.00 24.14	CPS1
ATOM	685	0	PRO	87	72.355	45.061	0.222	1.00 23.36	CPS1
ATOM	686	N	TYR	88	72.383	46.775	-1.223	1.00 23.09	CPS1
ATOM	687	CA	TYR	88	72.456	47.775	-0.170	1.00 22.80	CPS1
ATOM	688	CB	TYR	88	73.903	48.132	0.169	1.00 23.97	CPS1
ATOM	689	CG	TYR	88	74.662	48.796	-0.948	1.00 23.15	CPS1
ATOM	690	CD1	TYR	88	74.617	50.176	-1.121	1.00 23.81	CPS1
ATOM	691	CE1	TYR	88	75.334	50.803	-2.148	1.00 24.04	CPS1
ATOM	692	CD2	TYR	88	75.438	48.042	-1.823	1.00 23.00	CPS1
MOTA	693	CE2	TYR	88	76.163	48.653	-2.853	1.00 23.00	CPS1
ATOM	694	CZ	TYR	88	76.106	50.031	-3.007	1.00 24.59	CPS1
ATOM	695	OH	TYR	88	76.807	50.635	-4.029	1.00 23.69	CPS1
MOTA	696	С	TYR	88	71.697	48.978	-0.676	1.00 24.07	CPS1
ATOM	697	0	TYR	88	71.492	49.131	-1.882	1.00 24.63	CPS1
ATOM	698	N	ILE	89	71.265	49.821	0.247	1.00 23.90	CPS1
ATOM	699	CA	ILE	89	70.486	50.992	-0.096	1.00 24.96	CPS1
ATOM	700	CB	ILE	89	69.183	51.038	0.763	1.00 25.43	CPS1
ATOM	701		ILE	89	68.580	52:445	0.773	1.00 23.76	CPS1
ATOM	702	CG1		89	68.179	50.007	0.237	1.00 25.76	CPS1
ATOM	703			89	66.920	49.857	1.102	1.00 25.48	CPS1
ATOM	704	c	ILE	89	71.230	52.304	0.086	1.00 26.98	CPS1
ATOM	705	ō	ILE	89	72.018	52.470	1.020	1.00 27.02	CPS1
ATOM	706	N	ILE	90	70.984	53.227	-0.840	1.00 28.88	CPS1
ATOM	707	CA	ILE	90	71.543	54.567	-0.750	1.00 28.88	
ATOM	708	CB	ILE	90	72.383	54.968	-1.983	1.00 31.89	CPS1
ATOM	709	CG2		90	72.685	56.465	-1.930	1.00 34.32	CPS1
ATOM	710			90	73.692	54.176	-2.020	1.00 34.95	CPS1
ATOM	711		ILE	90	74.585	54.381	-0.812		CPS1
ATOM	712	C	ILE	90	70.299	55.433	-0.715	1.00 36.25	CPS1
ATOM	713	ō	ILE	90	69.450	55.342	-1.599	1.00 32.42	CPS1
ATOM	714	N	CYS	91	70.165	56.246	0.320		CPS1
ATOM	715	CA	CYS	91	69.002	57.106		1.00 32.73	CPS1
ATOM	716	CB	CYS	91	68.008	56.543	0.433	1.00 34.96	CPS1
ATOM	717	SG	CYS	91	66.523	57.557	1.463	1.00 32.49	CPS1
ATOM	718	c	CYS	91	69.452		1.657	1.00 29.59	CPS1
ATOM	719	ō	CYS	91	70.079	58.494	0.848	1.00 38.10	CPS1
ATOM	720	N	THR	92		58.666	1.893	1.00 40.46	CPS1
ATOM	721	CA	THR	92	69.124	59.476	0.014	1.00 42.14	CPS1
ATOM	722	CB	THR	92	69.489	60.870	0.246	1.00 45.56	CPS1
ATOM	723	OG1		92	68.964	61.772	-0.898	1.00 46.93	CPS1
ATOM	724		THR		67.552	61.562	-1.069	1.00 48.39	CPS1
ATOM	725	C	THR	92	69.686	61.454	-2.205	1.00 47.93	CPS1
ATOM	726	0	THR	92	69.001	61.457	1.571	1.00 46.35	CPS1
ATOM	727	N		92	69.345	62.592	1.901	1.00 47.51	CPS1
ATOM	728	CA	LYS LYS	93	68.211	60.703	2.332	1.00 46.09	CPS1
ATOM	729	CB		93	67.714	61.218	3.602	1.00 46.14	CPS1
ATOM	730	CG	LYS	93	66.214	60.944	3.725	1.00 46.87	CPS1
ATOM	731		LYS	93	65.395	61.870	2.837	1.00 48.42	CPS1
ATOM		CD	LYS	93	63.903	61.704	3.034	1.00 49.49	CPS1
ATOM	732	CE	LYS	93	63.148	62.908	2.482	1.00 50.63	CPS1
ATOM	733	NZ	LYS	93	63.471	63.177	1.054	1.00 52.22	CPS1
ATOM	734	C	LYS	93	68.452	60.733	4.844	1.00 45.50	CPS1
	735	0	LYS	93	68.167	61.182	5.954	1.00 45.52	CPS1
ATOM	736	N	LEU	94	69.408	59.829	4.657	1.00 44.83	CPS1
ATOM	737	CA	LEU	94	70.200	59.313	5.770	1.00 44.48	CPS1
ATOM	738	CB	LEU	94	69. 376	58.330	6.611	1.00 44.44	CPS1
ATOM	739	CG	LEU	94	68.488	57.283	5.928	1.00 44.15	CPS1
ATOM	740	CD1	LEA	94	69.258	56.498	4.886	1.00 42.30	CPS1



SEP 0 9 2002

FIG. 1A-13

0.G. FIG.	CLASS SUBCLASS	-	
APPROVED	À.	DRAFTSMAN	

ATOM	741		LEU	94	67.934	56.361	6.997	1.00 43.28	CPS
ATOM	742	С	LEU	94	71.486	58.641	5.307	1.00 44.30	CPSI
ATOM	743	0	LEU	94	71.692	58.432	4.111	1.00 44.84	CPSI
ATOM	744	N	SER	95	72.353	58.308	6.257	1.00 43.56	CPSI
ATOM	745	CA	SER	95	73.612	57.655	5.934	1.00 44.17	
ATOM	746	CB	SER	95	74.583	57.748	7.107	1.00 44.85	CPSI
ATOM	747	OG	SER	95	75.803	57.098	6.784		CPSI
ATOM	748	C	SER	95	73.408	56.184	5.577	1.00 47.82	CPS1
ATOM	749	ō	SER	95	72.676	55.462		1.00 43.59	CPSI
ATOM	750	N	PRO	96	74.065		6.258	1.00 43.06	CPS1
ATOM	751	CD	PRO	96	75.025	55.720	4.503	1.00 42.46	CPS1
ATOM	752	CA	PRO	96		56.444	3.650	1.00 42.90	CPS1
ATOM	753	CB	PRO	96	73.939	54.325	4.079	1.00 41.30	CPS1
ATOM	754	CG	PRO		74.757	54.286	2.788	1.00 42.08	CPS1
ATOM	755	C		96	75.821	55.316	3.045	1.00 42.41	CPS1
ATOM	756	0	PRO	96	74.473	53.379	5.153	1.00 39.30	CPS1
ATOM			PRO	96	74.098	52.210	5.206	1.00 38.17	CPS1
ATOM	757	N	ALA	97	75.348	53.901	6.008	1.00 37.86	CPS1
	758	CA	ALA	97	75.929	53.117	7.095	1.00 36.05	CPS1
ATOM	759	CB	ALA	97	76.982	53.940	7.819	1.00 37.73	CPS1
ATOM	760	С	ALA	97	74.857	52.681	8.090	1.00 35.10	CPS1
ATOM	761	0	ALA	97	74.992	51.662	8.770	1.00 35.38	CPS1
ATOM	762	N	ALA	98	73.789	53.460	8.173	1.00 33.38	CPS1
ATOM	763	CA	ALA	98	72.717	53.160	9.107	1.00 31.76	CPS1
ATOM	764	CB	ALA	98	72.057	54.454	9.546	1.00 33.83	CPS1
ATOM	765	C	ALA	98	71.657	52.220	8.537	1.00 30.24	CPS1
ATOM	766	0	ALA	98	70.734	51.849	9.255	1.00 31.14	CPS1
ATOM	767	N	VAL	99	71.796	51.831	7.269	1.00 26.77	CPS1
ATOM	768	CA	VAL	99	70.803	50.980	6.607	1.00 25.25	CPS1
ATOM	769	CB	VAL	99	70.258	51.695	5.331	1.00 24.54	CPS1
ATOM	770		VAL	99	69.091	50.920	4.731	1.00 24.61	CPS1
ATOM	771		VAL	99	69.829	53.107	5.676	1.00 26.14	CPS1
ATOM	772	С	VAL	99	71.272	49.576	6.207	1.00 23.74	CPS1
ATOM	773	0	VAL	99	72.390	49.393	5.720	1.00 23.55	CPS1
ATOM	774	N	HIS	100	70.395	48.595	6.422	1.00 22.48	CPS1
ATOM	775	CA	HIS	100	70.640	47.195	6.075	1.00 21.75	CPS1
ATOM	776	CB	HIS	100	70.873	46.360	7.334	1.00 23.99	CPS1
MOTA	777	CG	HIS	100	72.020	46.846	8.160	1.00 27.42	CPS1
ATOM	778	CD2	HIS	100	72.060	47.696	9.212	1.00 28.79	CPS1
ATOM	779	ND1	HIS	100	73.329	46.542	7.859	1.00 28.14	CPS1
ATOM	780	CE1	HIS	100	74.128	47.190	8.689	1.00 30.71	CPS1
ATOM	781	NE2	HIS	100	73.383	47.898	9.519	1.00 30.71	CPS1
ATOM	782	С	HIS	100	69.394	46.686	5.357	1.00 20.99	CPS1
ATOM	783	0	HIS	100	68.270	47.007	5.752	1.00 20.00	
ATOM	784	N	VAL	101	69.593	45.893	4.312	1.00 20.41	CPS1
ATOM	785	CA	VAL	101	68.473	45.357	3.551	1.00 20.41	CPS1
ATOM	786	CB	VAL	101	68.181	46.244	2.290	1.00 20.21	CPS1
ATOM	787	CG1	VAL	101	69.391	46.245	1.344		CPS1
ATOM	788		VAL	101	66.958	45.723	1.553	1.00 22.43	CPS1
ATOM	789	C	VAL	101	68.761	43.723		1.00 21.20	CPS1
ATOM	790	0	VAL	101	69.920		3.084	1.00 20.38	CPS1
ATOM	791	N	SER	102	67.702	43.527	2.986	1.00 19.26	CPS1
ATOM	792	CA	SER	102		43.167	2.835	1.00 19.19	CPS1
ATOM	793	СВ	SER	102	67.867	41.833	2.280	1.00 19.46	CPS1
ATOM	794	OG	SER	102	67.884	40.742	3.345	1.00 18.79	CPS1
ATOM	795	c .	SER	102	68.068	39.478	2.720	1.00 18.64	CPS1
ATOM	796	ō	SER	102	66.677	41.638	1.358	1.00 20.37	CPS1
ATOM	797	N	ILE	102	65.581	42.095	1.658	1.00 20.10	CPS1
			-115	103	66.902	40.964	0.236	1.00 19.92	CPS1



SEP 0 9 2002

FIG. 1A-14

ATOM	798	CA	ILE		65.847	40.737	-0.744	1.00 19.71	CPS1
ATOM	799	CB	ILE		66.122	41.550	-2.033	1.00 19.02	CPS1
ATOM	800		! ILE		64.988	41.337	-3.054	1.00 19.50	CPS1
ATOM	801		ILE		66.234	43.031	-1.682	1.00 18.90	CPS1
ATOM	802		. ILE		6 6.7 67	43.904	-2.828	1.00 19.01	CPS1
ATOM	8 0 3	С	ILE		65.804	39.265	-1.090	1.00 20.30	CPS1
ATOM	804	0	ILE		66.847	38.620	-1.164	1.00 20.97	CPS1
ATOM	805	N	THR		64.603	38.729	-1.287	1.00 20.48	CPS1
ATOM	806	CA	THR		64.468	37.316	-1.623	1.00 20.34	CPS1
ATOM	807	CB	THR		64.172	36.462	-0.350	1.00 21.86	CPS1
ATOM ATOM	808 809	CG2	THR	104	64.222	35.065	-0.671	1.00 21.77	CPS1
ATOM	810	C	THR	104	62.804	36.795	0.213	1.00 20.65	CPS1
ATOM	811		THR	104	63.346	37.139	-2.642	1.00 21.68	CPS1
ATOM	812	И	HIS	104	62.501	38.018	-2.813	1.00 20.50	CPS1
ATOM	813	CA	HIS	105 105	63.345	36.003	-3.325	1.00 22.11	CPS1
ATOM	814	CB	HIS	105	62.323	35.728	-4.331	1.00 24.82	CPS1
ATOM	815	CG	HIS	105	62.884	35.948	-5.747	1.00 27.53	CPS1
ATOM	816		HIS	105	63.383 64.585	37.335	-6.020	1.00 32.22	CPS1
ATOM	817		HIS	105	62.615	37.915 38.292	-5.782	1.00 34.13	CPS1
ATOM	818		HIS	105	63.322	39.402	-6.648	1.00 36.59	CPS1
ATOM	819		HIS	105	64.521	39.199	-6.786 -6.271	1.00 35.80	CPS1
ATOM	820	c	HIS	105	61.863	34.268	-4.280	1.00 35.22 1.00 24.66	CPS1
ATOM	821	o	HIS	105	62.570	33.400	-3.766	1.00 23.89	CPS1
ATOM	822	N	THR	106	60.667	34.027	-4.811	1.00 23.89	CPS1
ATOM	823	CA	THR	106	60.127	32.677	-5.003	1.00 24.24	CPS1
ATOM	824	CB	THR	106	59.008	32.271	-4.019	1.00 25.81	CPS1 CPS1
ATOM	825	OG1	THR	106	57.840	33.073	-4.253	1.00 25.01	CPS1
MOTA	826	CG2	THR	106	59.483	32.419	-2.570	1.00 24.51	CPS1
ATOM	827	С	THR	106	59.500	32.820	-6.388	1.00 25.67	CPS1
ATOM	828	0	THR	106	59.496	33.915	-6.953	1.00 25.60	CPS1
ATOM	829	N	ALA	107	58.962	31.740	-6.939	1.00 25.39	CPS1
MOTA	830	CA	ALA	107	58.355	31.824	-8.262	1.00 25.43	CPS1
ATOM	831	CB	ALA	107	57.743	30.463	-8.637	1.00 25.15	CPS1
ATOM	832	С	ALA	107	57.288	32.918	-8.363	1.00 25.95	CPS1
ATOM	833	0	ALA	107	57.233	33.660	-9.353	1.00 25.81	CPS1
ATOM	834	N	GLU	108	56.452	33.035	-7.335	1.00 24.82	CPS1
ATOM	835	CA	GLU	108	55.356	34.007	-7.367	1.00 25.17	CPS1
ATOM	836	CB	GLU	108	54.043	33.295	-7.008	1.00 27.79	CPS1
ATOM	837	CG	GLU	108	53.688	32.198	-8.005	1.00 34.77	CPS1
ATOM	838	CD	GLU	108	52.404	31.450	-7.675	1.00 39.77	CPS1
ATOM	839		GLU	108	52.146	30.431	-8.355	1.00 43.18	CPS1
ATOM	840	OE2	GLU	108	51.652	31.864	-6.758	1.00 42.25	CPS1
ATOM	841	С	GLU	108	55.486	35.267	-6.507	1.00 24.23	CPS1
ATOM	842	0	GLU	108	54.654	36.178	-6.615	1.00 22.93	CPS1
ATOM	843	N	TYR	109	56.518	35.330	-5.669	1.00 21.86	CPS1
ATOM ATOM	844	CA	TYR	109	56.678	36.480	-4.788	1.00 21.64	CPS1
ATOM	845 846	CB	TYR	109	56.320	36.077	-3.352	1.00 22.31	CPS1
ATOM	847	CG	TYR	109	54.889	35.632	-3.180	1.00 23.87	CPS1
ATOM	848		TYR	109	53.868	36.562	-2.999	1.00 23.05	CPS1
ATOM	849			109	52.546	36.164	-2.894	1.00 24.80	CPS1
ATOM	850	CD2 CE2	TYR	109	54.550	34.283	-3.253	1.00 24.86	CPS1
ATOM	851	CZ	TYR	109	53.226	33.872	-3.154	1.00 27.10	CPS1
ATOM	852	OH	TYR	109	52.233	34.818	-2.977	1.00 24.92	CPS1
ATOM	853	C	TYR	109	50.924	34.420	-2.916	1.00 25.87	CPS1
ATOM	854	0	TYR	109	58.066	37.100	-4.741	1.00 21.01	CPS1
	334	5	IIK	109	59.063	36.476	-5.091	1.00 21.94	CPS1



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-15

APPROVED [] G. F | G. ORAFISFANI

ATOM	855	N	ALA	110	58.097	38.347	-4.292	1.00 20.81	CPS1
ATOM	856	CA	ALA	110	59.344	39.074	-4.057	1.00 20.89	
ATOM	857	CB	ALA	110	59.483	40.256	-5.013		CPS1
ATOM	858		ALA					1.00 21.11	CPS1
		C		110	59.155	39.574	-2.617	1.00 19.96	CPS1
ATOM	859	0	ALA	110	58.043	39.941	-2.238	1.00 21.37	CPS1
ATOM	860	N	ALA	111	60.209	39.576	-1.805	1.00 18.57	CPS1
ATOM	861	CA	ALA	111	60.074	40.062	-0.435	1.00 17.40	CPS1
ATOM	862	CB	ALA	111	59.780	38.896	0.509	1.00 16.67	CPS1
ATOM	863	С	ALA	111	61.362	40.756	-0.023	1.00 17.97	CPS1
ATOM	864	0	ALA	111	62.411	40.476	-0.580	1.00 17.28	CPS1
ATOM	865	N	ALA	112	61.275	41.676	0.931	1.00 16.46	CPS1
ATOM	866	CA	ALA	112	62.458	42.374	1.394	1.00 17.56	CPS1
ATOM	867	CB	ALA	112	62.786	43.553	0.444	1.00 17.14	CPS1
ATOM	868	С	ALA	112	62.263	42.880	2.809	1.00 16.81	CPS1
ATOM	869	0	ALA	112	61.143	43.042	3.270	1.00 17.67	CPS1
ATOM	870	N	GLN	113	63.361	43.106	3.514	1.00 17.77	CPS1
ATOM	871	CA	GLN	113	63.267	43.639	4.863	1.00 17.77	CPS1
ATOM	872	CB	GLN	113	63.469	42.554	5.929	1.00 17.30	
ATOM	873	CG	GLN	113	64.842				CPS1
ATOM	874	CD	GLN			41.925	5.912	1.00 22.22	CPS1
ATOM	875	OE1		113	65.029	40.878	6.990	1.00 26.02	CPS1
ATOM				113	66.130	40.366	7.182	1.00 29.00	CPS1
	876	NE2		113	63.950	40.541	7.688	1.00 28.62	CPS1
ATOM	877	С	GLN	113	64.370	44.658	4.985	1.00 18.39	CPS1
ATOM	878	0	GLN	113	65.410	44.550	4.338	1.00 19.07	CPS1
ATOM	879	N	VAL	114	64.142	45.639	5.836	1.00 18.02	CPS1
ATOM	880	CA	VAL	114	65.128	46.675	6.042	1.00 17.24	CPS1
ATOM	881	CB	VAL	114	64.702	47.987	5.317	1.00 17.08	CPS1
ATOM	882		VAL	114	65.511	49.194	5.863	1.00 16.82	CPS1
ATOM	883	CG2	VAL	114	64.897	47.837	3.810	1.00 15.69	CPS1
ATOM	884	С	VAL	114	65.223	46.962	7.526	1.00 18.35	CPS1
ATOM	885	0	VAL	114	64.228	46.862	8.260	1.00 17.93	CPS1
ATOM	886	N	VAL	115	66.429	47.280	7.973	1.00 19.07	CPS1
ATOM	887	CA	VAL	115	66.622	47.702	9.351	1.00 20.05	CPS1
ATOM	888	CB	VAL	115	67.435	46.698	10.193	1.00 21.79	CPS1
ATOM	889	CG1	VAL	115	67.695	47.297	11.582	1.00 24.02	CPS1
ATOM	890	CG2	VAL	115	66.680	45.387	10.322	1.00 21.49	CPS1
ATOM	891	c	VAL	115	67.411	49.003	9.266	1.00 20.53	CPS1
ATOM	892	ō	VAL	115	68.416	49.077	8.552	1.00 19.46	
ATOM	893	N	ILE	116	66.921	50.038	9.943		CPS1
ATOM	894	CA	ILE	116	67.620			1.00 22.12	CPS1
ATOM	895	CB	ILE	116		51.321	9.987	1.00 22.75	CPS1
ATOM	896		ILE		66.694	52.492	9.629	1.00 22.88	CPS1
ATOM	897		ILE	116	67.430	53.825	9.850	1.00 23.51	CPS1
ATOM				116	66.232	52.353	8.172	1.00 22.44	CPS1
	898		ILE	116	65.208	53.382	7.742	1.00 20.81	CPS1
ATOM	899	C	ILE	116	68.090	51.495	11.430	1.00 25.25	CPS1
ATOM	900	0	ILE	116	67.312	51.296	12.363	1.00 22.08	CPS1
ATOM	901	N	GLU	117	69.362	51.845	11.610	1.00 28.24	CPS1
ATOM	902	CA	GLU	117	69.923	52.041	12.944	1.00 33.38	CPS1
ATOM	903	CB	GLU	117	71.297	51.384	13.074	1.00 34.32	CPS1
ATOM	904	CG	GLU	117	71.376	49.888	12.878	1.00 36.79	CPS1
ATOM	905	CD	GLU	117	72.808	49.388	13.006	1.00 38.57	CPS1
ATOM	906	OE1	GLU	117	73.266	49.163	14.144	1.00 40.54	CPS1
MOTA	907	OE2	GLU	117	73.489	49.243	11.971	1.00 40.35	CPS1
ATOM	908	С	GLU	117	70.119	53.524	13.216	1.00 36.51	CPS1
ATOM	909	0	GLU	117	70.269	54.317	12.289	1.00 36.14	CPS1
ATOM	910	N	ARG	118	70.120	53.890	14.493	1.00 40.58	CPS1
ATOM	911	CA	ARG	118	70.358	55.275	14.884	1.00 45.79	CPS1
					,0.336	33.275	44.004	1.00 45.79	CFSI



SEP 0 9 2002

FIG. 1A-16

G	SUBCLASS	
0.G. FI	51.ASS S	
APPROVED	÷ 63	DRAFTSHAN

ATOM	912	CB	ARG	118	69.712	55.600	16.235	1.00 46.59	CPS1
ATOM	913	CG	ARG	118	68.229	55.336	16.356	1.00 49.65	CPS1
ATOM	914	CD	ARG	118	67.792	55.527	17.809	1.00 52.26	CPS1
ATOM	915	NE	ARG	118	66.418	55.092	18.046	1.00 54.79	CPS1
ATOM	916	CZ	ARG	118	65.337	55.786	17.702	1.00 55.39	CPS1
ATOM	917	NH1	. ARG	118	64.131	55.299	17.956	1.00 56.47	CPS1
ATOM	918	NH2	ARG	118	65.458	56.972	17.120	1.00 56.32	CPS1
ATOM	919	C	ARG	118	71.868	55.331	15.069	1.00 48.09	CPS1
ATOM	920	0	ARG	118	72.435	54.481	15.755	1.00 49.38	CPS1
ATOM	921	N	LEU	119	72.529	56.308	14.462	1.00 50.93	CPS1
ATOM	922	CA	LEU	119	73.973	56.418	14.631	1.00 53.26	CPS1
ATOM	923	CB	LEU	119	74.651	56.655	13.277	1.00 53.81	CPS1
ATOM	924	CG	LEU	119	74.474	55.541	12.239	1.00 54.33	CPS1
ATOM	925	CD1	LEU	119	75.203	55.906	10.953	1.00 54.92	CPS1
ATOM	926		LEU	119	75.006	54.234	12.801	1.00 54.83	CPS1
ATOM	927	C	LEU	119	74.286	57.568	15.591	1.00 54.83	
MOTA	928		LEU	119	74.613	57.278	16.765	1.00 55.09	CPS1
ATOM	929		LEU	119	74.177	58.740	15.166		CPS1
ATOM	930	C	GLY	0	77.740	47.623	17.259	1.00 55.10	CPS1
ATOM	931	ō	GLY	ŏ	78.476	48.184		1.00 45.52	CPS2
ATOM	932	N	GLY	ŏ	79.569	47.872	16.444	1.00 47.54	CPS2
ATOM	933	CA	GLY	0	78.237		18.959	1.00 47.48	CPS2
ATOM	934	N	GLY	1	76.484	47.280	18.650	1.00 46.63	CPS2
ATOM	935	CA	GLY	i	75.916	47.284	16.983	1.00 43.42	CPS2
ATOM	936	c	GLY	1		47.570	15.679	1.00 38.90	CPS2
ATOM	937	0	GLY	1	75.631	46.308	14.888	1.00 35.36	CPS2
ATOM	938	N	ILE		76.138	45.233	15.198	1.00 35.52	CPS 2
ATOM				2	74.818	46.451	13.853	1.00 32.81	CPS 2
ATOM	939	CA	ILE	2	74.444	45.331	12.997	1.00 30.92	CPS 2
ATOM	940	CB	ILE	2 ·	73.034	45.554	12.419	1.00 30.17	CPS2
ATOM	941		ILE	2	72.715	44.495	11.369	1.00 28.15	CPS 2
ATOM	942		ILE	2	72.019	45.547	13.564	1.00 30.04	CPS2
ATOM	943		ILE	2	70.624	45.977	13.162	1.00 29.29	CPS2
	944	C	ILE	2	75.427	45.143	11.851	1.00 30.22	CPS2
ATOM	945	0	ILE	2	75.785	46.098	11.157	1.00 29.17	CPS2
ATOM	946	N	TYR	3	75.866	43.906	11.657	1.00 29.82	CPS2
ATOM	947	CA	TYR	3	76.797	43.596	10.577	1.00 29.72	CPS2
ATOM	948	CB	TYR	3	77.594	42.334	10.900	1.00 32.80	CPS2
ATOM	949	CG	TYR	3	78.536	41.959	9.782	1.00 37.46	CPS2
ATOM	950		TYR	3	79.553	42.827	9.394	1.00 39.59	CPS2
ATOM	951		TYR	3	80.382	42.538	8.314	1.00 42.43	CPS2
ATOM	952		TYR	3	78.370	40.775	9.064	1.00 39.81	CPS2
ATOM	953		TYR	3	79.196	40.470	7.974	1.00 42.42	CPS2
ATOM	954	CZ	TYR	3	80.201	41.364	7.607	1.00 44.04	CPS2
ATOM	955	OH	TYR	3	81.024	41.099	6.531	1.00 46.34	CPS2
ATOM	956	С	TYR	3	76.032	43.379	9.275	1.00 28.30	CPS2
ATOM	957	0	TYR	3	76.420	43.872	8.211	1.00 28.24	CPS2
ATOM	958	N	GLY	4	74.944	42.619	9.363	1.00 25.87	CPS2
ATOM	959	CA	GLY	4	74.141	42.355	8.182	1.00 22.75	CPS2
ATOM	960	С	GLY	4	72.849	41.652	8.547	1.00 21.62	CPS2
ATOM	961	0	GLY	4	72.724	41.085	9.639	1.00 21.41	CPS2
ATOM	962	N	ILE	5	71.877	41.703	7.640	1.00 20.89	CPS2
ATOM	963	CA	ILE	5	70.593	41.042	7.859	1.00 19.45	
ATOM	964	CB	ILE	5	69.453	42.057	8.118	1.00 19.45	CPS2 CPS2
ATOM	965	CG2	ILE	5	69.846	43.011	9.259	1.00 18.65	
ATOM	966	CG1		5	69.129	42.843		1.00 19.69	CPS2
ATOM	967	CD1		5	67.947		6.842		CPS2
ATOM	968	c	ILE	5		43.809	7.020	1.00 20.64	CPS2
		_		,	70.272	40.216	6.618	1.00 18.82	CPS2



RECEIVED SEP 0 9 2002

FIG. 1A-17

-16.	SUBCLASS	
10.G.F	CLASS	
APPROVED.	ž	DRAFTSMAH

MOTA	969	0	ILE	5	70.778	40.498	5.524	1.00 18.88	CPS2
ATOM	970	N	GLY	6	69.456	39.184	6.794	1.00 19.17	CPS2
ATOM	971	CA	GLY	6	69.108	38.325	5.679	1.00 19.31	CPS2
ATOM	972	С	GLY	6	67. 6 87	37.815	5.794	1.00 19.36	CPS2
ATOM	973	0	GLY	6	67.176	37.614	6.887	1.00 18.63	CPS2
ATOM	974	N	LEU	7	67.053	37.606	4.649	1.00 19.78	CPS2
ATOM	975	CA	LEU	7	65.680	37.141	4.617	1.00 19.08	CPS2
ATOM	976	CB	LEU	7	64.733	38.328	4.366	1.00 19.19	CPS2
ATOM	977	CG	LEU	7	63.238	38.018	4.161	1.00 18.29	CPS2
ATOM	978		LEU	7	62.658	37.539	5.491	1.00 18.90	CPS2
ATOM	979		LEU	7	62.472	39.269	3.651	1.00 17.44	CPS2
ATOM	980	c	LEU	7	65.552	36.139	3.487	1.00 18.38	CPS2
ATOM	981	ō	LEU	7	66.113	36.338	2.417	1.00 19.54	CPS2
ATOM	982	N	ASP	8	64.845	35.042	3.724	1.00 18.51	CPS2
ATOM	983	CA	ASP	8	64.651	34.091	2.647	1.00 20.25	CPS2
ATOM	984	CB	ASP	8	65.727	32.998	2.657	1.00 20.25	CPS2
ATOM	985	CG	ASP	8	65.487	31.943	1.580	1.00 25.13	CPS2
ATOM	986		ASP	8	64.777	30.949			
ATOM	987		ASP	8	65.989	32.124	1.851	1.00 25.80	CPS2
ATOM	988	C	ASP	8	63.297	32.124	0.454	1.00 28.14	CPS2
ATOM							2.740	1.00 20.84	CPS2
ATOM	989	0	ASP	8	62.826	33.137	3.834	1.00 19.86	CPS2
	990	N	ILE	9	62.669	33.223	1.584	1.00 19.61	CPS2
ATOM ATOM	991	CA	ILE	9	61.391	32.520	1.533	1.00 20.19	CPS2
	992	CB	ILE	9	60.222	33.393	1.015	1.00 21.26	CPS2
ATOM	993		ILE	9	58.9 5 0	32.526	0.904	1.00 20.13	CPS2
ATOM	994	CG1	ILE	9	59.959	34.555	1.973	1.00 21.42	CPS2
ATOM	995		ILE	9	58.878	35.500	1.490	1.00 21.37	CPS2
ATOM	996	С	ILE	9	61.641	31.415	0.519	1.00 20.37	CPS2
ATOM	997	0	ILE	9	62.132	31.685	-0.572	1.00 20.53	CPS2
ATOM	998	N	THR	10	61.313	30.182	0.892	1.00 20.80	CPS2
ATOM	999	CA	THR	10	61.519	29.032	0.022	1.00 22.14	CPS2
ATOM	1000	CB	THR	10	62.584	28.076	0.630	1.00 23.02	CPS2
ATOM	1001	OG1		10	63.837	28.770	0.746	1.00 25.04	CPS2
ATOM	1002	CG2	THR	10	62.785	26.859	-0.253	1.00 25.37	CPS2
ATOM	1003	С	THR	10	60.211	28.275	-0.184	1.00 21.99	CPS2
MOTA	1004	0	THR	10	59.471	28.038	0.761	1.00 21.01	CPS2
ATOM	1005	N	GLU	11	59.938	27.912	-1.435	1.00 23.31	CPS2
ATOM	1006	CA	GLU	11	58.723	27.177	-1.794	1.00 24.42	CPS2
ATOM	1007	CB	GLU	11	58.438	27.355	-3.296	1.00 26.52	CPS2
ATOM	1008	CG	GLU	11	57.052	26.900	-3.721	1.00 28.30	CPS2
ATOM	1009	CD	GLU	11	56.897	26.756	-5.231	1.00 32.57	CPS2
ATOM	1010	OE1	GLU	11	57.820	27.134	-5.991	1.00 32.18	CPS2
ATOM	1011	OE2	GLU	11	55.833	26.256	-5.654	1.00 33.69	CPS2
MOTA	1012	С	GLU	11	58.941	25.692	-1.480	1.00 23.56	CPS2
MOTA	1013	0	GLU	11	59.853	25.070	-2.026	1.00 22.90	CPS2
MOTA	1014	N	LEU	12	58.110	25.124	-0.612	1.00 23.91	CPS2
MOTA	1015	CA	LEU	12	58.260	23.715	-0.249	1.00 26.06	CPS2
ATOM	1016	CB	LEU	12	57.147	23.269	0.705	1.00 28.23	CPS2
ATOM	1017	CG	LEU	12	57.554	23.114	2.176	1.00 31.10	CPS2
ATOM	1018	CD1	LEU	12	58.046	24.448	2.710	1.00 30.63	CPS2
ATOM	1019		LEU	12	56.360	22.605	3.005	1.00 32.22	CPS2
ATOM	1020	С	LEU	12	58.271	22.795	-1.461	1.00 27.56	CPS2
ATOM	1021	ō	LEU	12	59.054	21.846	-1.519	1.00 27.33	CPS2
ATOM	1022	N	ALA	13	57.401	23.077	-2.427	1.00 27.64	CPS2
ATOM	1023	CA	ALA	13	57.321	22.255	-3.628	1.00 27.84	CPS2
ATOM	1024	CB	ALA	13	56.163			1.00 28.61	CPS2
ATOM	1025	c	ALA	13	58.622	22.714	-4.506	1.00 28.81	CPS2
	2023	-	· 1111	13	50.622	22.279	-4.413	1.00 29.21	CPS2



SEP 0 9 2002

FIG. 1A-18

(i	SUBCLASS	
J.G. F10	CLASS ISU	-
APPROVED	7.2	DRAFTSHAH

MOTA	1026	0	ALA	13	58.982	21.281	-5.048	1.00 28.52	CPS2
ATOM	1027	N	ARG	14	59.335	23.404	-4.375	1.00 29.11	CPS2
ATOM	1028	CA	ARG	14	60.599	23.495	-5.098	1.00 30.50	CPS2
ATOM	1029	CB	ARG	14	61.065	24.951	-5.221	1.00 32.06	CPS2
ATOM	1030	CG	ARG	14	62.248	25.118	-6.171	1.00 34.92	CPS2
ATOM	1031	CD	ARG	14	62.528	26.576	-6.477	1.00 36.22	CPS2
ATOM	1032	NE	ARG	14	63.217	27.245		1.00 38.47	
ATOM	1033	CZ	ARG	14	64.522	27.137			CPS2
ATOM	1033		ARG					1.00 39.99	CPS2
				14	65.284	26.385		1.00 39.47	CPS2
ATOM	1035		ARG	14	65.066	27.787		1.00 39.80	CPS2
ATOM	1036	C	ARG	14	61.670	22.655	-4.411	1.00 30.84	CPS2
ATOM	1037	0	ARG	14	62.488	22.021		1.00 31.28	CPS2
ATOM	1038	N	ILE	15	61.672	22.650		1.00 31.04	CPS2
ATOM	1039	CA	ILE	15	62.637	21.845		1.00 31.02	CPS2
ATOM	1040	CB	ILE	15	62.480	22.037	-0.803	1.00 30.76	CPS2
ATOM	1041	CG2	ILE	15	63.314	21.002	-0.056	1.00 29.83	CPS2
ATOM	1042	CG1	ILE	15	62.940	23.441	-0.407	1.00 29.97	CPS2
ATOM	1043	CD1	ILE	15	64.431	23.685	-0.657	1.00 30.60	CPS2
ATOM	1044	С	ILE	15	62.397	20.369	-2.673	1.00 33.28	CPS2
ATOM	1045	0	ILE	15	63.338	19.604	-2.900	1.00 33.51	CPS2
ATOM	1046	N	ALA	16	61.133	19.974	-2.712	1.00 34.78	CPS2
ATOM	1047	CA	ALA	16	60.789	18.597		1.00 37.29	CPS2
ATOM	1048	СВ	ALA	16	59.285	18.395	-2.921	1.00 37.29	
ATOM	1049	c	ALA	16	61.264	18.286	-4.459	1.00 39.28	CPS2
ATOM	1050	0	ALA	16					CPS2
ATOM	1050	N			61.839	17.230	-4.716	1.00 40.75	CPS2
			SER	17	61.034	19.219		1.00 40.88	CPS2
ATOM	1052	CA	SER	17	61.439	19.046	-6.763	1.00 43.46	CPS2
ATOM	1053	CB	SER	17	61.012	20.261	-7.588	1.00 44.13	CPS2
ATOM	1054	OG	SER	17	61.450	20.150		1.00 46.75	CPS2
ATOM	1055	С	SER	17	62.949	18.857	-6.866	1.00 44.93	CPS2
ATOM	1056	0	SER	17	63.432	18.058	-7.672	1.00 44.94	CPS2
ATOM	1057	N	MET	18	63.694	19.597	-6.052	1.00 45.72	CPS2
ATOM	1058	CA	MET	18	65.148	19.499	-6.060	1.00 47.01	CPS2
ATOM	1059	CB	MET	18	65.780	20.713	-5.374	1.00 47.40	CPS2
ATOM	1060	CG	MET	18	65.783	21.978	-6.201	1.00 48.61	CPS2
ATOM	1061	SD	MET	18	66.874	23.231	-5.488	1.00 51.56	CPS2
ATOM	1062	CE	MET	18	65.856	23.843	-4.148	1.00 49.70	CPS2
ATOM	1063	С	MET	18	65.637	18.233	-5.369	1.00 47.60	CPS2
ATOM	1064	0	MET	18	66.589	17.605	-5.822	1.00 48.05	CPS2
ATOM	1065	N	ALA	19	64.982	17.863	-4.275	1.00 48.91	CPS2
ATOM	1066	CA	ALA	19	65.365	16.682	-3.512	1.00 50.86	CPS2
ATOM	1067	CB	ALA	19	64.590	16.637	-2.209	1.00 50.39	CPS2
ATOM	1068	c	ALA	19	65.135				
ATOM	1069	ō	ALA/		65.897	15.396	-4.296	1.00 53.04	CPS2
ATOM	1070	N	GLY	20		14.433	-4.171	1.00 52.81	CPS2
ATOM	1071	CA	GLY		64.084	15.384	-5.108	1.00 54.91	CPS2
ATOM	1071			20	63.773	14.201	-5.888	1.00 56.86	CPS2
ATOM		C	GLY	20	64.693	13.980	-7.072	1.00 58.24	CPS2
	1073	0	GLY	20	65.285	12.90 9	-7.217	1.00 58.99	CPS2
ATOM	1074	N	ARG	21	64.827	14.996	-7.916	1.00 59.32	CPS2
ATOM	1075	CA	ARG	21	65.652	14.882	-9.107	1.00 60.71	CPS2
ATOM	1076	CB	ARG	21	65.279	15.975	-10.112	1.00 61.88	CPS2
ATOM	1077	CG	ARG	21	65.739	17.362	-9.716	1.00 63.83	CPS2
ATOM	1078	CD	ARG	21	65.818	18.274	-10.930	1.00 65.39	CPS2
ATOM	1079	NE	ARG	21	66.617	19.471	-10.669	1.00 67.17	CPS2
ATOM	1080	CZ	ARG	21	66.250	20.467	-9.867	1.00 67.54	CPS2
ATOM	1081	NH1	ARG	21	65.082	20.423	-9.237	1.00 68.19	CPS2
ATOM	1082		ARG	21	67.057	21.507	-9.693	1.00 67.30	CPS2
					07.057	21.50/	-9.693	1.00 67.30	CPSZ







ATOM

1083 C

1004

FIG. 1A-19

ARG 21

200

67.153 14.932 -8.857 1.00 61.11 CPS2

APPROYED O.G. FIG.

ATOM	1084	0	ARG	21	67.942	14.571	-9.735	1.00 61.28	CPS2
ATOM	1085	N	GLN	22	67.564	15.375	-7.674	1.00 61.25	CPS2
ATOM	1086	CA	GLN	22	68.994	15.461	-7.402	1.00 60.88	CPS2
ATOM	1087	CB	GLN	22	69.340	16.826	-6.795	1.00 61.70	CPS2
ATOM	1088	CG	GLN	22	69.033	17.998	-7.722	1.00 62.47	
ATOM	1089	CD	GLN	22	69.522	19.331	-7.180		CPS2
MOTA	1090	OE1		22				1.00 63.25	CPS2
ATOM	1091	NE2	GLN	22	69.279	20.381	-7.779	1.00 63.34	CPS2
					70.218	19.297	-6.047	1.00 63.02	CPS2
ATOM	1092	С	GLN	22	69.563	14.351	-6.530	1.00 60.08	CPS2
ATOM	1093	0	GLN	22	68.836	13:608	-5.867	1.00 60.33	CPS2
ATOM	1094	N	LYS	23	70.886	14.253	-6.569	1.00 59.12	CPS2
ATOM	1095	CA	LYS	23	71.665	13.273	-5.823	1.00 57.97	CPS2
ATOM	1096	CB	LYS	23	73.137	13.684	-5.890	1.00 59.44	CPS2
ATOM	1097	CG	LYS	23	73.362	15.214	-5.851	1.00 60.21	CPS2
ATOM	1098	CD	LYS	23	73.057	15.850	-4.501	1.00 59.91	CPS2
ATOM	1099	CE	LYS	23	73.391	17.340	-4.455	1.00 60.70	CPS2
ATOM	1100	NZ	LYS	23	72.466	18.181	-5.268	1.00 59.44	CPS2
MOTA	1101	С	LYS	23	71.253	13.118	-4.360	1.00 56.31	CPS2
ATOM	1102	0	LYS	23	70.226	12.517	-4.027	1.00 57.13	CPS2
ATOM	1103	N	ARG	24	72.112	13.635	-3.496	1.00 53.19	CPS2
ATOM	1104	CA	ARG	24	71.909	13.629	-2.062	1.00 50.41	CPS2
ATOM	1105	CB	ARG	24	73.117	12.987	-1.365	1.00 51.60	CPS2
ATOM	1106	CG	ARG	24	74.311	12.739	-2.286	1.00 51.00	CPS2
ATOM	1107	CD	ARG	24	75.442	12.014	-1.565	1.00 52.64	
ATOM	1108	NE	ARG	24	75.142				CPS2
ATOM	1109	CZ	ARG	24	75.534	9.570	-1.218	1.00 51.83	CPS2
ATOM	1110		ARG				-1.892	1.00 51.87	CPS2
ATOM	1111			24	76.318	9.728	-2.950	1.00 51.30	CPS2
ATOM			ARG	24	75.187	8.347	-1.505	1.00 51.09	CPS2
	1112	C	ARG	24	71.787	15.110	-1.717	1.00 47.01	CPS2
MOTA	1113	0	ARG	24	72.640	15.690	-1.043	1.00 46.57	CPS2
ATOM	1114	N	PHE	25	70.725	15.721	-2.238	1.00 42.31	CPS2
MOTA	1115	CA	PHE	25	70.450	17.134	-2.019	1.00 38.57	CPS2
ATOM	1116	CB	PHE	25	69.115	17.508	-2.679	1.00 37.72	CPS2
MOTA	1117	CG	PHE	25	68.680	18.926	-2.416	1.00 36.40	CPS2
ATOM	1118		PHE	25	67.682	19.202	-1.485	1.00 36.71	CPS2
MOTA	1119		PHE	25	69.285	19.986	-3.080	1.00 37.10	CPS2
ATOM	1120	CEl	PHE	25	67.297	20.518	-1.220	1.00 36.02	CPS2
ATOM	1121	CE2	PHE	25	68.910	21.305	-2.824	1.00 35.88	CPS2
ATOM	1122	CZ	PHE	25	67.914	21.572	-1.891	1.00 36.06	CPS2
ATOM	1123	С	PHE	25	70.415	17.465	-0.528	1.00 36.15	CPS2
ATOM	1124	0	PHE	25	71.053	18.423	-0.079	1.00 35.69	CPS2
ATOM	1125	N	ALA	26	69.671	16.664	0.228	1.00 33.10	CPS2
ATOM	1126	CA	ALA	26	69.548	16.865	1.667	1.00 32.04	CPS2
ATOM	1127	CB	ALA	26	68.663	15.780	2.270	1.00 30.86	CPS2
ATOM	1128	C	ALA	26	70.931	16.835	2.312		
ATOM	1129	ō	ALA	26	71.249	17.655		1.00 31.57	CPS2
ATOM	1130	N	GLU	27	71.747		3.180	1.00 28.07	CPS2
ATOM	1131	CA	GLU	27		15.881	1.868	1.00 29.98	CPS2
ATOM	1132	CB	GLU	27	73.102	15.717	2.382	1.00 30.25	CPS2
ATOM	1133	CG	GLU		73.745	14.457	1.794	1.00 31.17	CPS2
ATOM				27	73.219	13.134	2.356	1.00 35.24	CPS2
	1134	CD	GLU	27	71.772	12.823	1.978	1.00 37.65	CPS2
ATOM	1135		GLU	27	71.300	13.296	0.918	1.00 38.95	CPS2
ATOM	1136		GLU	27	71.113	12.076	2.742	1.00 40.73	CPS2
ATOM	1137	С	GLU	27	73.974	16.925	2.063	1.00 28.88	CPS2
ATOM	1138	0	GLU	27	74.879	17.254	2.823	1.00 28.66	CPS2
ATOM	1139	И	ARG	28	73.705	17.578	0.935	1.00 27.77	CPS2



SEP 0 9 2002

TECH CENTER 1600/2900

SEP 8 3 2002 N

ATOM

1187 OG

1188 C

1190 N

1191 CA

1192 CB

1195 OE1 GLU

1196 OE2 GLU

1189

1193 CG GLU

1194 CD GLU

33

33

33

34

34

34

34

34

34

34

SER

SER

GLU

GLU

GLU

74.402

72.345

71.036

71.178

71.493

71.939

71.813

72.427

72.464 16.813

71.488 16.317

18.784

17.682

18.051

19.215

20.554

21.642

13.645

12.652

13.211

11.654

11.131

10.140

10.824

9.860

22.838 10.220 1.00 26.38

21.310 8.755 1.00 25.66

1.00 37.61

1.00 28.59

1.00 27.50

1.00 27.39

1.00 27.27

1.00 26.09

1.00 27.08

1.00 27.39

CPS2

	ATOM	1140	CA	ARG	28	74.470	18.754	0.532	1.00 29.47	CPS2
	ATOM	1141	CB	ARG	28	74.201	19.076	-0.948	1.00 30.98	CPS2
	ATOM	1142	CG	ARG	28	74.785	20.407	-1.424	1.00 35.00	CPS2
SS	ATOM	1143	CD	ARG	28	74.806	20.528	-2.953	1.00 38.43	CPS2
1 15 1	ATOM	1144	NE	ARG	28	73.480	20.654	-3.557	1.00 40.71	CPS2
1.418	ATOM	1145	CZ	ARG	28	72.809	21.797	-3.683	1.00 42.27	CPS2
F1G.	ATOM	1146	NH1	ARG	28	73.327	22.940	-3.248	1.00 42.45	CPS2
100	ATOM	1147		ARG	28	71.613	21.798	-4.259	1.00 44.17	CPS2
0.6. F	ATOM	1148	c	ARG	28	74.137	19.987	1.387	1.00 28.50	CPS2
lold	ATOM	1149	ō	ARG	28	75.003	20.811	1.669	1.00 29.58	CPS2
The state of the same of	ATOM	1150	N	ILE	29	72.879	20.105	1.788	1.00 26.47	CPS2
¥ ¥	ATOM	1151	CA	ILE	29	72.426	21.256	2.570	1.00 26.47	CPS2
g > 2	ATOM	1152	СВ	ILE	29	70.908	21.475	2.389	1.00 25.79	
APPROVES 6Y ORAFTSMAH	ATOM	1153		ILE	29	70.467	22.729	3.147		CPS2
ا ا	ATOM	1154		ILE	29	70.559	21.566	0.902	1.00 24.32	CPS2
	ATOM	1155		ILE	29	71.283	22.665		1.00 23.95	CPS2
	ATOM	1156	CDI					0.158	1.00 26.12	CPS2
	ATOM	1156	0	ILE	29	72.681	21.128	4.064	1.00 26.65	CPS2
				ILE	29	73.024	22.110	4.739	1.00 26.47	CPS2
	ATOM	1158	N	LEU	30	72.516	19.908	4.566	1.00 26.29	CPS2
	ATOM	1159	CA	LEU	30	72.638	19.616	5.981	1.00 26.30	CPS2
	ATOM	1160	CB	LEU	30	71.518	18.645	6.371	1.00 26.05	CPS2
	ATOM	1161	CG	LEU	30	70.095	19.059	5.957	1.00 26.30	CPS2
	ATOM	1162		LEU	30	69.081	18.002	6.387	1.00 26.56	CPS2
	ATCH	1163		LEU	30	69.762	20.400	6.602	1.00 24.24	CPS2
	ATOM	1164	С	LEU	30	73.972	19.075	6.497	1.00 27.26	CPS2
	ATOM	1165	0	LEU	30	74.731	18.419	5.771	1.00 28.28	CPS 2
	MOTA	1166	N	THR	31	74.246	19.372	7.765	1.00 26.23	CPS2
	ATOM	1167	CA	THR	31	75.451	18.898	8.434	1.00 26.09	CPS2
	ATOM	1168	CB	THR	31	75.844	19.806	9.627	1.00 24.78	CPS2
	MOTA	1169	OG1		31	74.834	19.723	10.638	1.00 25.44	CPS2
	MOTA	1170		THR	31	75.998	21.253	9.172	1.00 25.52	CPS2
	ATOM	1171	С	THR	31	75.106	17.516	8.978	1.00 26.34	CPS2
	ATOM	1172	0	THR	31	73.945	17.106	8.956	1.00 25.24	CPS2
	ATOM	1173	N	ARG	32	76.108	16.791	9.463	1.00 28.14	CPS2
	MOTA	1174	CA	ARG	32	75.8 7 2	15.456	10.005	1.00 30.16	CPS2
	ATOM	1175	CB	ARG	32	77.195	14.862	10.519	1.00 32.90	CPS2
	ATOM	1176	CG	ARG	32	77.070	13.518	11.243	1.00 37.77	CPS2
	ATOM	1177	CD	ARG	32	78.452	13.018	11.667	1.00 42.29	CPS2
	MOTA	1178	NE	ARG	32	78.428	12.082	12.796	1.00 46.64	CPS2
	ATOM	1179	CZ	ARG	32	78.020	10.817	12.728	1.00 48.51	CPS2
	ATOM	1180	NH1	ARG	32	77.588	10.314	11.581	1.00 50.24	CPS2
	ATOM	1181	NH2	ARG	32	78.058	10.045	13.809	1.00 49.25	CPS2
	ATOM	1182	С	ARG	32	74.812	15.450	11.116	1.00 29.69	CPS2
	ATOM	1183	0	ARG	32	73.946	14.577	11.149	1.00 29.33	CPS2
	ATOM	1184	N	SER	33	74.858	16.428	12.019	1.00 29.98	CPS2
	ATOM	1185	CA	SER	33	73.886	16.473	13.112	1.00 29.46	CPS2
	ATOM	1186	CB	SER	33	74.338	17.475	14.180	1.00 32.61	CPS2
	7 TOM	1107		000		72.330	27.475	14.100	1.00 32.01	CPSZ



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-21

25F 0.3 5005 F

1197 C

GLU

ATOM

OLASS SUBCLASS

ATOM	1197	C GLU	34
ATOM	1198	O GLU	34
ATOM	1199	N LEU	35
MOTA	1200	CA LEU	35
ATOM	1201	CB LEU	35
ATOM	1202	CG LEU	35
ATOM	1202	CD1 LEU	35
MOTA	1204	CD2 LEU	35
ATOM	1205	C LEU	35
ATOM	1206	O LEU	35
ATOM	1207	N ASP	36
MOTA	1208	CA ASP	36
ATOM	1209	CB ASP	36
ATOM	1210	CG ASP	36
MOTA	1211	OD1 ASP	36
ATOM	1212	OD2 ASP	36
ATOM	1213	C ASP	36
ATOM	1214	O ASP	36
ATOM	1215	N GLN	37
			37
ATOM	1216		
ATOM	1217	CB GLN	37
ATOM	1218	CG GLN	37
ATOM	1219	CD GLN	37
MOTA	1220	OE1 GLN	37
ATOM	1221	NE2 GLN	37
MOTA	1222	C GLN	37
ATOM	1223	O GLN	37
ATOM	1224	N TYR	38
ATOM	1225	CA TYR	38
ATOM	1226	CB TYR	38
ATOM	1227	CG TYR	38
ATOM			38
ATOM	1228 1229	CD1 TYR	38
		CE1 TYR	
ATOM	1230	CD2 TYR	38
ATOM	1231	CE2 TYR	38
MOTA	1232	CZ TYR	38
MOTA	1233	OH TYR	38
ATOM	1234	C TYR	38
ATOM	1235	O TYR	38
ATOM	1236	N TYR	39
ATOM	1237	CA TYR	39
ATOM	1238	CB TYR	39
ATOM	1239	CG TYR	39
ATOM	1240	CD1 TYR	39
ATOM	1241	CE1 TYR	39
ATOM	1241	CD2 TYR	39
ATOM			
	1243	CE2 TYR	39
MOTA	1244	CZ TYR	39
MOTA	1245	OH TYR	39
MOTA	1246	C TYR	39
ATOM	1247	O TYR	39
ATOM	1248	N GLU	40
ATOM	1249	CA GLU	40
ATOM	1250	CB GLU	40
ATOM	1251	CG GLU	40
ATOM	1252	CD GLU	40
ATOM	1253	OE1 GLU	40
211OF	1233	OEI GEO	40

70.443	16.828	10.437	1.00 27.36	CPS2
69.239	16.562	10.532	1.00 26.33	CPS2
71.302	16.077	9.750	1.00 28.28	CPS2
70.862	14.877	9.045	1.00 29.11	CPS2
72.021	14.251	8.270	1.00 28.46	CPS2
72.336	14.922	6.940	1.00 27.65	CPS2
73.659	14.380	6.379	1.00 27.03	CPS2
71.182	14.664	5.965	1.00 28.02	CPS2
70.281	13.851	9.998	1.00 30.80	CPS2
69.303	13.191	9.668	1.00 31.95	CPS2
70.883	13.709	11.175	1.00 32.92	CPS2
70.380	12.756	12.161	1.00 35.31	CPS2
71.247	12.759	13.416	1.00 38.59	CPS2
72.527	11.974	13.236	1.00 43.41	CPS2
72.449	10.838	12.713	1.00 47.13	CPS2
73.606	12.480	13.618	1.00 45.83	CPS2
68.948	13.107	12.531	1.00 35.32	CPS2
68.108	12.228	12.733	1.00 35.28	CPS2
68.675	14.404	12.621	1.00 34.28	CPS2
67.338	14.881	12.945	1.00 32.79	CPS2
67.401	16.378	13.297	1.00 33.92	CPS2
68.022	16.651	14.662	1.00 35.15	CPS2
68.443	18.110	14.876	1.00 36.52	CPS2
68.733	18.517	16.001	1.00 37.53	CPS2
68.495	18.887	13.799	1.00 34.94	CPS2
66.431	14.645	11.733	1.00 32.14	CPS2
65.284	14.214	11.863	1.00 31.52	CPS2
66.971	14.914	10.552	1.00 30.64	CPS2
66.239	14.753	9.307	1.00 30.51	CPS2
67.112	15.245	8.148	1.00 29.87	CPS2
66.544	15.040	6.762	1.00 30.29	CPS2
66.975	13.983	5.957	1.00 31.01	CPS2
66.500	13.829	4.653	1.00 31.49	CPS2
65.614	15.935	6.231	1.00 30.83	CPS2
65.135	15.792	4.938	1.00 31.82	CPS2
65.582	14.742	4.153	1.00 32.74	CPS2
65.116	14.623	2.868	1.00 33.33	CPS2
65.802 64.631	13.308	9.064 8.773	1.00 31.79 1.00 30.55	CPS2 CPS2
66.739	12.372	9.190	1.00 30.55	CPS2
66.423	10.965	8.946	1.00 33.46	CPS2
67.675	10.096	9.077	1.00 33.46	CPS2
68.760	10.350	8.045	1.00 30.99	CPS2
68.449	10.548	6.702	1.00 31.00	CPS2
69.458	10.707	5.744	1.00 31.73	CPS2
70.108	10.321	8.413	1.00 32.22	CPS2
71.125	10.474	7.468	1.00 32.57	CPS2
70.795	10.665	6.137	1.00 32.96	CPS2
71.813	10.784	5.211	1.00 33.59	CPS2
65.331	10.411	9.862	1.00 34.30	CPS2
64.653	9.451	9.506	1.00 35.26	CPS2
65.155	11.015	11.030	1.00 36.00	CPS2
64.144	10.555	11.980	1.00 38.47	CPS2
64.468	11.069	13.387	1.00 41.11	CPS2
65.650	10.394	14.052	1.00 46.35	CPS2
65.427	8.903	14.247	1.00 49.30	CPS2

15.006 1.00 50.90

64.505

8.527

CPS2



RECEIVED

SEP 0 9 2002

FIG. 1A-22

Γ	455	
9	SUBCLASS	
C.	L.ASS	
(Q)	ΙΞ	77 × 72
APPROVE	÷	DRAFISMAN

MOTA	1254	OE2	GLU	40	66.174	8.108	13.632	1.00 51.72	CPS2
ATOM	1255	С	GLU	40	62.720	10.980	11.631	1.00 38.59	CPS2
ATOM	1256	0	GLU	40	61.761	10.472	12.210	1.00 38.70	CPS2
MOTA	1257	N	LEU	41	62.579	11.905	10.688	1.00 37.33	CPS2
ATOM	1258	CA	LEU	41	61.262	12.409	10.318	1.00 37.21	CPS2
ATOM	1259	CB	LEU	41	61.371	13.881	9.908	1.00 36.12	CPS2
ATOM	1260	CG	LEU	41	61.978	14.843	10.928	1.00 35.44	CPS2
ATOM	1261	CD1	LEU	41	62.095	16.224	10.296	1.00 35.33	CPS2
ATOM	1262	CD2	LEU	41	61.110	14.897	12.175	1.00 36.15	CPS2
ATOM	1263	С	LEU	41	60.540	11.653	9.210	1.00 37.79	CPS2
ATOM	1264	0	LEU	41	61.147	10.905	8.441	1.00 37.84	CPS2
ATOM	1265	N	SER	42	59.231	11.882	9.130	1.00 38.99	CPS2
ATOM	1266	CA	SER	42	58.394	11.272	8.105	1.00 39.66	CPS2
ATOM	1267	CB	SER	42	56.916	11.461	8.451	1.00 40.41	CPS2
ATOM	1268	OG	SER	42	56.529	12.813	8.277	1.00 40.55	CPS2
ATOM	1269	С	SER	42	58.688	11.947	6.769	1.00 40.88	CPS2
ATOM	1270	0	SER	42	59.404	12.948	6.716	1.00 40.22	CPS2
ATOM	1271	N	GLU	43	58.118	11.405	5.698	1.00 41.38	CPS2
ATOM	1272	CA	GLU	43	58.310	11.948	4.358	1.00 41.99	CPS2
ATOM	1273	CB	GLU	43	57.466	11.173	3.340	1.00 44.33	CPS2
ATOM	1274	CG	GLU	43	56.922	9.822	3.821	1.00 47.83	CPS2
ATOM	1275	CD	GLU	43	55.963	9.946	5.005	1.00 50.30	CPS2
ATOM	1276			43	55.186	10.935	5.055	1.00 50.62	CPS2
ATOM	1277		GLU	43	55.982	9.045	5.877	1.00 48.97	CPS2
ATOM	1278	c	GLU	43	57.921	13.425	4.294	1.00 40.64	CPS2
ATOM	1279	ō	GLU	43	58.662	14.259	3.767	1.00 40.30	CPS2
ATOM	1280	N	LYS	44	56.747	13.739	4.825	1.00 39.19	CPS2
ATOM	1281	CA	LYS	44	56.249	15.112	4.821	1.00 39.31	CPS2
ATOM	1282	CB	LYS	44	54.787	15.140	5.269	1.00 40.00	CPS2
ATOM	1283	CG	LYS	44	54.112	16.491	5.107	1.00 42.53	CPS2
ATOM	1284	CD	LYS	44	52.721	16.472	5.719	1.00 44.55	CPS2
ATOM	1285	CE	LYS	44	52.031	17.817	5.592	1.00 45.48	CPS2
ATOM	1286	NZ	LYS	44	50.783	17.861	6.406	1.00 47.64	CPS2
ATOM	1287	C	LYS	44	57.075	16.023	5.732	1.00 38.50	CPS2
ATOM	1288	ō	LYS	44	57.446	17.136	5.345	1.00 38.08	CPS2
ATOM	1289	N	ARG	4.5	57.345	15.554	6.947	1.00 36.81	CPS2
ATOM	1290	CA	ARG	45	58.125	16.335	7.898	1.00 36.28	CPS2
ATOM	1291	CB	ARG	45	58.162	15.624	9.254	1.00 37.98	CPS2
ATOM	1292	CG	ARG	45	56.911	15.843	10.106	1.00 37.98	CPS2
ATOM	1293	CD	ARG	45	57.135	16.960	11.117	1.00 45.38	CPS2
ATOM	1294	NE	ARG	45	57.655	18.160	10.468	1.00 49.29	CPS2
ATOM	1295	cz	ARG	45	58.565	18.968	11.002	1.00 49.81	CPS2
ATOM	1296		ARG	45	59.064	18.714	12.206	1.00 51.08	CPS2
ATOM	1297		ARG	45	58.993	20.022	10.323	1.00 50.35	CPS2
ATOM	1298	C	ARG	45	59.537	16.595	7.382	1.00 34.46	CPS2
ATOM	1299	ō	ARG	45	60.105	17.657	7.629	1.00 34.48	CPS2
ATOM	1300	N	LYS	46	60.107	15.630	6.662	1.00 33.18	CPS2
ATOM	1301	CA	LYS	46	61.444	15.814	6.110	1.00 32.44	
ATOM	1302	CB	LYS	46	61.891				CPS2
ATOM	1303	CG	LYS	46	62.375	14.589 13.419	5.295 6.133	1.00 32.49	CPS2
ATOM	1304	CD	LYS	46	62.872	12.296	5.245	1.00 33.28	CPS2 CPS2
ATOM	1305	CE	LYS	46	63.389	11.131	6.065	1.00 34.31	
ATOM	1306	NZ	LYS	46	63.700				CPS2
ATOM	1307	c	LYS	46		9.994	5.169	1.00 36.69	CPS2
ATOM	1308	0	LYS	46	61.479	17.039	5.206	1.00 31.46	CPS2
ATOM	1309	N	ASN	47	62.393	17.856	5.290	1.00 31.48	CPS2
ATOM	1310	CA	ASN	47	60.481	17.163	4.336	1.00 30.42	CPS2
	2320	-	.1011	*/	60.417	18.286	3.407	1.00 31.16	CPS2

SEP 0 9 2002

FIG. 1A-23

TECH CENTER 1600/2900

CPS2

CPS 2

CPS2

CPS2

CPS2

CPS2

CPS2

CPS2

SUBCLASS CLASS

ATOM 1311 CB ASN 47 ATOM 1312 CG ASN 47 47 ATOM 1313 OD1 ASN ATOM 1314 MD2 ASN 47 47 ATOM 1315 C ASN ATOM 1316 0 ASN 47 ATOM 1317 CLU 48 N ATOM 1318 CA GLU 48 ATOM 1319 CB GLU 48 ATOM 1320 CG GLU 48 ATOM 1321 CD GLU 48 ATOM 1322 OE1 GLU 48 ATOM 1323 OES GLU 48 ATOM 1324 C GLU 48 ATOM 1325 GLU 48 ATOM 1326 N PHE 49 ATOM 1327 CA PHE 49 ATOM 1328 CB PHE 49 ATOM 1329 CG PHE 49 ATOM 1330 CD1 PHE 49 ATOM 1331 CD2 PHE 49 ATOM 1332 CE1 PHE 49 ATOM 1333 CE₂ PHE 49 ATOM 1334 CZ PHE 49 ATOM 49 1335 C PHE ATOM 1336 0 PHE 49 ATOM 1337 N LEU 50 ATOM 1338 CA LEU 50 ATOM 1339 CB LEU 50 ATOM 1340 CG LEU 50 ATOM 1341 CDI LEU 50 ATOM 1342 CD2 LEU 50 ATOM 1343 С LEU 50 ATOM 1344 LEU 0 ATOM 1345 N ALA 51 ATOM 1346 CA ALA ATOM 1347 CB AT.A 51 ATOM 1348 С ALA 51 ATOM 1349 O AT.A ATOM 1350 GLY 52 ATOM 1351 CA GLY 52 ATOM 1352 C GLY 52 ATOM 1353 0 GT.V 52 ATOM 1354 ARG 53 ATOM 1355 CA ARG 53 ATOM 1356 CB ARG 53 ATOM 1357 CG ARG 53 ATOM 1358 CD ARG 53 ATOM 1359 NE ARG 53 ATOM 1360 C7. ARG 53 ATOM 1361 NH1 ARG 53 ATOM 1362 NH2 ARG 53 ATOM 1363 C ARG 53 ATOM 1364 0 ARG 53 ATOM 1365 N PHE 54 ATOM 1366 CA PHE 54 ATOM 1367 CB PHE 54

59.240 18.101 2.437 1.00 32.45 59.080 19.269 1.470 1.00 34.97 59.977 19.575 0.684 1.00 37.44 57.928 19.923 1.525 1.00 35.87 60.290 19.612 4.157 1.00 29.73 60.946 20.587 1.00 28.79 3.803 59.462 19.637 5.195 1.00 28.89 59.265 20.853 5.984 1.00 29.80 58.162 20.642 7.019 1.00 32.74 56.837 20.225 6.424 1.00 37.62 55.785 19.953 7.482 1.00 40.29 54.683 19.506 7.113 1.00 41.90 56.059 20.193 8.679 1.00 42.74 60.554 21.231 6.700 1.00 28.72 60.956 22.396 6.720 1.00 27.50 61.192 20.230 7.296 1.00 26.72 62.432 20.433 8.023 1.00 26.17 62.877 19.116 8.665 1.00 27.12 64.186 19.205 9.397 1.00 26.24 64.219 19.514 10.750 1.00 27.02 65.385 18.967 8.734 1.00 28.35 65.429 19.578 11.436 1.00 27.13 66.603 19.030 9.411 1.00 27.87 66.615 19.336 10.770 1.00 27.13 63.522 20.935 7.091 1.00 24.61 64.208 21.907 7.390 1.00 24.60 63.685 20.266 5.957 1.00 23.67 64.710 20.650 5.000 1.00 23.23 64.763 19.626 3.862 1.00 24.17 65.810 19.767 2.758 1.00 26.00 67.217 19.817 3.351 1.00 25.89 65.685 18.570 1.810 1.00 26.96 64.465 22.053 4.448 1.00 23.30 65.391 22.849 4.317 1.00 22.85 63.218 22.366 4.127 1.00 21.99 62.914 23.684 3.586 1.00 21.37 61.438 23.766 3.206 1.00 19.49 63.262 24.772 4.610 1.00 19.95 63.812 25.815 4.252 1.00 19.91 62.943 24.508 5.871 1.00 20.32 63.207 25.466 6.939 1.00 20.53 64.690 25.678 7.161 1.00 21.59 65.140 26.823 7.292 1.00 20.12 65.452 24.581 7.211 1.00 20.75 66.900 24.681 7.405 1.00 21.49 67.511 23.289 7.639 1.00 20.94 67.662 22.904 9.121 1.00 21.90 66.357 23.082 9.905 1.00 23.39 66.538 22,829 11.335 1.00 24.30 65.666 23.195 12.272 1.00 25.08 64.548 23.827 11.934 1.00 25.43 65.921 22.959 13.551 1.00 26.80 67.541 25.359 6.201 1.00 20.90 68.447 26.176 6.353 1.00 20.27 67.069 25.021 5.002 1.00 20.29 67.583 25.631 3.779 1.00 21.05 66.889 24.996 2.550 1.00 21.38



SEP 0 9 2002

FIG. 1A-24



ATOM	1368	CG	PHE	54	67.310	25.573	1.218	1.00 22.85	CPS2
ATOM	1369	CDI	PHE	54	6 6 .623	26.646	0.660	1.00 23.51	CPS2
ATOM	1370	CD2	PHE	54	68.363	25.008	0.495	1.00 23.11	CPS2
ATOM	1371	CEI	PHE	54	66.970	27.148	-0.600	1.00 23.62	CPS2
ATOM	1372	CE2	PHE	54	68.716	25.499	-0.761	1.00 24.74	CPS2
ATOM	1373	CZ	PHE	54	68.015	26.575	-1.313	1.00 24.84	CPS2
ATOM	1374	С	PHE	54	67.334	27.144	3.823	1.00 20.71	
ATOM	1375	0	PHE	54	68.225	27.939	3.523	1.00 20.71	CPS2
ATOM	1376	N	ALA	55	66.118	27.542	4.191	1.00 20.44	CPS2
ATOM	1377	CA	ALA	55	65.772	28.967	4.268	1.00 20.38	CPS2
ATOM	1378	CB	ALA	55	64.299	29.138	4.665		CPS2
ATOM	1379	C	ALA	55	66.654	29.701	5.276	1.00 19.50	CPS2
ATOM	1380	ō	ALA	55	67.111	30.822	5.021	1.00 20.15	CPS2
ATOM	1381	N	ALA	56	66.872	29.071		1.00 19.68	CPS2
ATOM	1382	CA	ALA	56	67.706	29.657	6.428	1.00 20.22	CPS2
ATOM	1383	CB	ALA	56	67.670		7.476	1.00 19.63	CPS2
ATOM	1384	C	ALA	56	69.152	28.772	8.737	1.00 20.93	CPS2
ATOM	1385	ō	ALA	56		29.841	7.014	1.00 20.43	CPS2
ATOM	1386	N	LYS	57	69.780	30.869	7.307	1.00 19.00	CPS2
ATOM	1387	CA			69.702	28.840	6.322	1.00 19.36	CPS2
ATOM	1388	CB	LYS	57	71.084	28.955	5.858	1.00 19.89	CPS2
ATOM			LYS	57	71.622	27.598	5.388	1.00 19.91	CPS2
ATOM	1389	CG	LYS	57	71.595	26.550	6.501	1.00 20.56	CPS2
ATOM	1390	CD	LYS	57	72.389	25.285	6.150	1.00 21.63	CPS2
	1391	CE	LYS	57	72.426	24.334	7.358	1.00 20.15	CPS2
ATOM	1392	NZ	LYS	57	73.457	23.262	7.208	1.00 19.99	CPS2
ATOM	1393	C	LYS	57	71.176	29.993	4.754	1.00 19.82	CPS2
ATOM	1394	0	LYS	57	72.136	30.755	4.698	1.00 20.57	CPS2
ATOM	1395	N	GLU	58	70.179	30.036	3.871	1.00 18.71	CPS2
ATOM	1396	CA	GLU	58	70.187	31.045	2.822	1.00 20.25	CPS2
ATOM	1397	CB	GLU	58	68.993	30.868	1.870	1.00 23.44	CPS2
ATOM	1398	CG	GLU	58	69.120	29.710	0.871	1.00 28.15	CPS2
ATOM	1399	CD	GLU	58	70.261	29.896	-0.124	1.00 31.42	CPS2
MOTA	1400	OE1	GLU	58	70.713	31.042	-0.335	1.00 33.78	CPS2
ATOM	1401	OE2	GLU	58	70.701	28.891	-0.713	1.00 35.13	CPS2
ATOM	1402	С	GLU	58	70.116	32.436	3.477	1.00 20.06	CPS2
ATOM	1403	0	GLU	58	70.878	33.335	3.117	1.00 20.02	
ATOM	1404	N	ALA	59	69.203	32.611	4.433	1.00 18.56	CPS2
ATOM	1405	CA	ALA	59	69.066	33.901	5.107	1.00 19.36	CPS2
ATOM	1406	CB	ALA	59	67.919	33.853	6.142		CPS2
ATOM	1407	C	ALA	59	70.388	34.280		1.00 18.28	CPS2
ATOM	1408	0	ALA	59	70.833	35.429	5.789 5.712	1.00 19.60	CPS2
ATOM	1409	N	PHE	60	71.016			1.00 20.42	CPS2
ATOM	1410	CA	PHE	60	72.284	33.314	6.452	1.00 18.99	CPS2
ATOM	1411	CB	PHE	60		33.591	7.119	1.00 19.29	CPS2
ATOM	1412	CG	PHE	60	72.790	32.350	7.862	1.00 20.46	CPS2
ATOM	1413		PHE		74.128	32.555	8.501	1.00 21.05	CPS2
ATOM	1414		PHE	60	74.225	33.085	9.785	1.00 21.57	ÇP\$2
ATOM	1415	CE1		60	75.297	32.313	7.783	1.00 23.12	CPS2
ATOM	1416			60	75.476	33.377	10.343	1.00 22.68	CPS2
ATOM		CE2		60	76.554	32.605	8.332	1.00 22.55	CPS2
ATOM	1417 1418	cz	PHE	60	76.638	33.136	9.610	1.00 22.82	CPS2
		C	PHE	60	73.338	34.020	6.092	1.00 20.21	CPS2
ATOM	1419	0	PHE	60	74.089	34.965	6.320	1.00 19.97	CPS2
ATOM	1420	N	SER	61	73.396	33.318	4.960	1.00 20.80	CPS2
ATOM	1421	CA	SER	61	74.372	33.641	3.920	1.00 20.87	CPS2
ATOM	1422	CB	SER	61	74.287	32.633	2.762	1.00 21.27	CPS2
ATOM	1423	OG	SER	61	73.161	32.874	1.942	1.00 22.46	CPS2
ATOM	1424	С	SER	61	74.190	35.058	3.389	1.00 21.75	CPS2
							3.309	22.73	CF32



SEP 0 9 2002 TECH CENTER 1600/2900

.G. F1G.	LASS SUBCLASS	
APPROVED (\.\.\.\.\.\.\.\.\.\.\.\.\.\.\.\.\.\.\.	DRAFTSMAN

ATOM	1425	0	SER	61	75.161	35.709	2.981	1.00 22.83	CPS2
ATOM	1426	N	LYS	62	72.949	35.541	3.396	1.00 20.78	CPS2
ATOM	1427	CA	LYS	62	72.657	36.890	2.934	1.00 21.54	CPS2
ATOM	1428	CB	LYS	62	71.158	37.027	2.627	1.00 22.99	CPS2
ATOM	1429	CG	LYS	62	70.696	36.164	1.444	1.00 27.37	
ATOM	1430	CD	LYS	62	69.195	35.912	1.505	1.00 30.44	CPS2
ATOM	1431	CE	LYS	62	68.439	36.617			CPS2
ATOM	1432	NZ	LYS	62	68.581		0.401	1.00 33.74	CPS2
ATOM	1433	C	LYS	62		35.960	-0.917	1.00 35.02	CPS2
ATOM					73.084	37.922	3.985	1.00 22.13	CPS2
	1434	0	LYS	62	73.546	39.009	3.638	1.00 22.23	CPS2
ATOM	1435	N	ALA	63	72.929	37.581	5.264	1.00 21.23	CPS2
ATOM	1436	CA	ALA	63	73.329	38.488	6.335	1.00 20.30	CPS2
ATOM	1437	CB	ALA	63	72.813	37.988	7.694	1.00 21.99	CPS2
ATOM	1438	C	ALA	63	74.851	38.541	6.337	1.00 22.63	CPS2
ATOM	1439	0	ALA	63	75.439	39.604	6.541	1.00 22.47	CPS2
ATOM	1440	N	PHE	64	75.473	37.387	6.092	1.00 23.43	CPS2
MOTA	1441	CA	PHE	64	76.934	37.257	6.040	1.00 26.03	CPS2
MOTA	1442	CB	PHE	64	77.315	35.788	5.814	1.00 28.19	
ATOM	1443	CG	PHE	64	78.780	35.482	6.042		CPS2
ATOM	1444		PHE	64	79.301			1.00 31.14	CPS2
ATOM	1445		PHE			35.418	7.329	1.00 33.14	CPS2
ATOM	1446		PHE	64	79.624	35.224	4.965	1.00 32.47	CPS2
ATOM				64	80.652	35.094	7.545	1.00 34.43	CPS2
	1447		PHE	64	80.969	34.900	5.163	1.00 33.63	CPS2
ATOM	1448	CZ	PHE	64	81.484	34.834	6.457	1.00 33.53	CPS2
ATOM	1449	С	PHE	64	77.481	38.136	4.905	1.00 27.97	CPS2
ATOM	1450	0	PHE	64	78.645	38.549	4.935	1.00 29.10	CPS2
ATOM	1451	N	GLY	65	76.642	38.388	3.901	1.00 28.14	CPS2
ATOM	1452	CA	GLY	65	76.999	39.256	2.786	1.00 29.01	CPS2
ATOM	1453	С	GLY	65	77.588	38.652	1.523	1.00 30.18	CPS2
ATOM	1454	0	GLY	65	77.945	39.377	0.596	1.00 31.12	CPS2
ATOM	1455	N	THR	66	77.660	37.332	1.454	1.00 30.26	
ATOM	1456	CA	THR	66	78.268	36.684	0.302		CPS2
ATOM	1457	СВ	THR	66	79.499	35.898		1.00 30.90	CPS2
ATOM	1458		THR	66	79.078		0.744	1.00 30.61	CPS2
ATOM	1459		THR	66		34.838	1.607	1.00 32.42	CPS2
ATOM	1460				80.457	36.790	1.525	1.00 31.71	CPS2
ATOM		C	THR	66	77.362	35.697	-0.410	1.00 31.06	CPS2
	1461	0	THR	66	77.601	35.355	~1.573	1.00 32.11	CPS2
ATOM	1462	N	GLY	67	76.332	35.232	0.288	1.00 30.08	CPS2
ATOM	1463	CA	GLY	67	75.460	34.226	-0.285	1.00 29.32	CPS2
ATOM	1464	С	GLY	67	76.230	32.923	-0.146	1.00 29.07	CPS2
MOTA	1465	0	GLY	67	77.357	32.929	0.354	1.00 28.18	CPS2
ATOM	1466	N	ILE	68	75.640	31.809	-0.566	1.00 29.24	CPS2
ATOM	1467	CA	ILE	68	76.315	30.518	-0.477	1.00 30.11	CPS2
ATOM	1468	CB	ILE	68	75.293	29.347	-0.467	1.00 29.33	CPS2
ATOM	1469	CG2	ILE	68	76.018	28.010	-0.446	1.00 29.51	CPS2
ATOM	1470	CG1		68	74.388	29.434	0.769	1.00 28.22	
ATOM	1471	CD1		68	75.100	29.195			CPS2
ATOM	1472	c	ILE	68			2.089	1.00 25.10	CPS2
ATOM	1473	ō	ILE	68	77.237	30.385	-1.697	1.00 32.39	CPS2
ATOM	1474	N	GLY		76.831	30.654	-2.827	1.00 32.91	CPS2
ATOM	1475			69	78.476	29.979	-1.460	1.00 32.97	CPS2
		CA	GLY	69	79.419	29.834	-2.552	1.00 35.33	CPS2
ATOM	1476	C	GLY	69	80.810	29.564	-2.028	1.00 36.14	CPS2
ATOM	1477	0	GLY	69	80.970	28.924	-0.992	1.00 36.01	CPS2
ATOM	1478	N	ALA	70	81.814	30.065	-2.742	1.00 37.62	CPS2
ATOM	1479	CA	ALA	70	83.212	29.872	-2.379	1.00 38.31	CPS2
ATOM	1480	CB	ALA	70	84.110	30.468	-3.473	1.00 38.64	CPS2
ATOM	1481	С	ALA	70	83.577	30.474	-1.025	1.00 38.65	CPS2
					,	-0.1.4	1.025	2.00 30.03	CF3Z



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SEP 0 9 2002

FIG. 1A-26

Γ	ASS	7
F16	S SUBCLASS	
0.0	CLASS	
APPROVE	40	DRAFTSHA

ATOM	1482	0	ALA	70	84.488	29.999	-0.345	1.00 39.72	CPS2
ATOM	1483	N	GLN	71	82.858	31.515	-0.628	1.00 38.67	CPS2
ATOM	1484	CA	GLN	71	83.130	32.197	0.630	1.00 37.32	CPS2
ATOM	1485	CB	GLN	71	82.744	33.666	0.472	1.00 40.43	CPS2
ATOM	1486	CG	GLN	71	83.693	34.659	1.118	1.00 44.57	CPS2
ATOM	1487	CD	GLN	71	83.654	36.018	0.431	1.00 46.06	CPS2
ATOM	1488	OE1	GLN	71	84.175	37.004	0.952	1.00 48.20	CPS2
ATOM	1489	NE2	GLN	71	83.044	36.069	-0.754	1.00 47.40	CPS2
ATOM	1490	С	GLN	71	82.391	31.578	1.824	1.00 35.81	CPS2
ATOM	1491	0	GLN	71	82.851	31.656	2.962	1.00 36.15	CPS2
ATOM	1492	N	LEU	72	81.257	30.944	1.561	1.00 32.57	CPS2
ATOM	1493	CA	LEU	72	80.461	30.353	2.630	1.00 30.34 .	CPS2
MOTA	1494	CB	LEU	72	79.503	31.400	3.196	1.00 29.93	CPS2
ATOM	1495	CG	LEU	72	78.560	30.935	4.303	1.00 29.85	CPS2
ATOM	1496	CD1	LEU	72	79.352	30.712	5.585	1.00 29.87	CPS2
ATOM	1497	CD2	LEU	72	77.482	31.998	4.515	1.00 30.13	CPS2
ATOM	1498	С	LEU	72	79.670	29.165	2.117	1.00 28.96	CPS2
ATOM	1499	0	LEU	72	78.925	29.270	1.146	1.00 29.65	CPS2
ATOM	1500	N	SER	73	79.828	28.037	2.791	1.00 26.89	CPS2
ATOM	1501	CA	SER	73	79.163	26.805	2.405	1.00 26.28	CPS2
ATOM	1502	CB	SER	73	80.176	25.656	2.498	1.00 27.70	CPS2
ATOM	1503	OG	SER	73	79.571	24.385	2.324	1.00 31.43	CPS2
ATOM	1504	C	SER	73	77.970	26.491	3.300	1.00 25.59	CPS2
ATOM	1505	0	SER	73	77.912	26.952	4.441	1.00 23.26	CPS2
ATOM	1506	11	PHE	74	77.016	25.718	2.780	1.00 24.61	CPS2
ATOM	1507	CA	PHE	74	75.874	25.292	3.591	1.00 24.32	CPS2
ATOM	1508	CB	PHE	74	74.974	24.333	2.813	1.00 24.91	CPS2
ATOM	1509	CG	PHE	74	74.016	25.012	1.887	1.00 27.32	CPS2
ATOM	1510		PHE	74	73.041	25.873	2.385	1.00 26.95	CPS2
ATOM	1511		PHE	74	74.079	24.787	0.511	1.00 28.10	CPS2
ATOM	1512		PHE	74	72.142	26.501	1.528	1.00 28.03	CPS2
ATOM	1513		PHE	74	73.185	25.411	-0.350	1.00 29.15	CPS2
ATOM	1514	CZ	PHE	74	72.214	26.271	0.160	1.00 27.71	CPS2
ATOM	1515	c	PHE	74	76.433	24.527	4.788	1.00 25.14	CPS2
ATOM	1516	ō	PHE	74	75.841	24.490	5.868	1.00 23.71	CPS2
ATOM	1517	N	GLN	75	77.577	23.886	4.571	1.00 25.71	CPS2
ATOM	1518	CA	GLN	75	78.212	23.099	5.618	1.00 26.61	CPS2
ATOM	1519	CB	GLN	75	79.212	22.115	4.998	1.00 26.65	CPS2
ATOM	1520	CG	GLN	75	78.580	21.089	4.063	1.00 27.20	CPS2
ATOM	1521	CD	GLN	75	77.513	20.259	4.742	1.00 26.33	CPS2
ATOM	1522		GLN	75	77.695	19.797	5.864	1.00 26.93	CPS2
ATOM	1523		GLN	75	76.390	20.057	4.056	1.00 27.72	CPS2
ATOM	1524	С	GLN	75	78.918	23.944	6.674	1.00 27.72	CPS2
ATOM	1525	ō	GLN	75	79.380	23.413	7.684	1.00 30.23	CPS2
ATOM	1526	N	ASP	76	79.020	25.250	6.455	1.00 28.01	CPS2
ATOM	1527	CA	ASP	76	79.676	26.113	7.441	1.00 26.83	CPS2
ATOM	1528	СВ	ASP	76	80.334	27.317	6.769	1.00 28.83	CPS2
ATOM	1529	CG	ASP	76	81.508	26.933	5.900	1.00 29.80	CPS2
ATOM	1530		ASP	76	82.291	26.066	6.330	1.00 29.26	CPS2
ATOM	1531		ASP	76	82.291	27.514	4.800	1.00 29.26	CPS2
ATOM	1532	C	ASP	76	78.657			1.00 30.74	CPS2
ATOM	1533	0	ASP	76		26.648	8.429		
ATOM	1534	N	ILE	77	79.015	27.306	9.412	1.00 26.97	CPS2 CPS2
ATOM	1535	CA	ILE	77	77.389	26.352	8.164	1.00 26.05	
ATOM	1536	CB	ILE	77	76.280	26.859	8.970	1.00 25.04	CPS2
ATOM	1537		ILE	77	75.306	27.678	8.079	1.00 23.67	CPS2 CPS2
ATOM	1538		ILE	77	74.270	28.414	8.942	1.00 24.94	
-11011	1230	CGI	TUE	,,	76.085	28.674	7.218	1.00 23.77	CPS2



SEP 0 9 2002

TECH CENTER 1600/2900



ATOM	1539	CD1	ILE	7 7	75.276	29.187	6.019	1.00 23.94	CPS2
ATOM	1540	С	ILE	7 7	75.487	25.717	9.586	1.00 25.85	CPS2
ATOM	1541	0	ILE	77	75.0 7 7	24.796	8.887	1.00 26.62	CPS2
ATOM	1542	N	GLU	78	75.260	25.7 7 3	10.892	1.00 24.57	CPS2
ATOM	1543	CA	GLU	78	74.483	24.727	11.529	1.00 24.12	CPS2
ATOM	1544	CB	GLU	78	75.366	23.875	12.450	1.00 24.96	CPS2
ATOM	1545	CG	GLU	78	74.631	22.661	13.039	1.00 26.74	CPS2
ATOM	1546	CD	GLU	78	75.579	21.638	13.643	1.00 30.06	CPS2
ATOM	1547	OE1	GLU	78	75.989	21.815	14.805	1.00 30.41	CPS2
ATOM	1548	OE2	GLU	78	75.930	20.656	12.942	1.00 30.57	CPS2
ATOM	1549	С	GLU	78	73.314	25.285	12.326	1.00 25.19	CPS2
ATOM	1550	0	GLU	78	73.467	26.243	13.096	1.00 24.62	CPS2
ATOM	1551	N	ILE	79	72.139	24.697	12.124	1.00 23.01	CPS2
ATOM	1552	CA	ILE	79	70.969	25.113	12.866	1.00 22.64	CPS2
ATOM	1553	CB	ILE	79	69.673	25.081	12.014	1.00 23.46	CPS2
ATOM	1554	CG2	ILE	79	68.519	25.648	12.832	1.00 25.86	CPS2
ATOM	1555		ILE	79	69.868	25.835	10.688	1.00 25.21	CPS2
ATOM	1556	CD1		79	70.337	27.256	10.820	1.00 27.02	CPS2
ATOM	1557	C	ILE	79	70.832	24.078	13.970	1.00 27.02	
ATOM	1558	0	ILE	79	70.679	22.882	13.691	1.00 22.93	CPS2
ATOM	1559	N	ARG	80	70.912	24.524	15.217	1.00 22.93	CPS2
ATOM	1560	CA	ARG	80	70.765	23.624	16.348		CPS2
ATOM	1561	CB	ARG	80	71.928	23.793	17.322	1.00 23.25	CPS2
ATOM	1562	CG	ARG	80	73.275	23.474		1.00 22.55	CPS2
ATOM	1563	CD	ARG	80	74.373	23.461	16.692	1.00 22.62	CPS2
ATOM	1564	NE	ARG	80	75.680		17.742	1.00 22.35	CPS2
ATOM	1565	cz	ARG	80	76.820	23.201	17.147	1.00 21.40	CPS2
ATOM	1566		ARG	80	76.820	23.280	17.823	1.00 22.68	CPS2
ATOM	1567		ARG	80	77.971	23.614	19.110	1.00 20.04	CPS2
ATOM	1568	C	ARG	80	69.456	23.020	17.216	1.00 22.34	CPS2
ATOM	1569	0	ARG	80		23.947	17.044	1.00 24.16	CPS2
ATOM	1570	и	LYS	81	68.837	24.965	16.757	1.00 23.92	CPS2
ATOM	1571	CA	LYS	81	69.028	23.074	17.947	1.00 26.40	CPS2
ATOM	1572	СВ	LYS		67.789	23.290	18.684	1.00 27.93	CPS2
ATOM	1573	CG	LYS	81	66.840	22.108	18.466	1.00 30.60	CPS2
ATOM	1574	CD	LYS	81	66.517	21.865	17.000	1.00 32.31	CPS2
ATOM	1575	CE		81	65.759	20.561	16.767	1.00 36.54	CPS2
ATOM	1576	NZ	LYS	81	64.326	20.645	17.248	1.00 39.00	CPS2
ATOM			LYS	81	63.553	19.423	16.848	1.00 41.89	CPS2
ATOM	1577	C	LYS	81	68.113	23.428	20.168	1.00 28.77	CPS2
ATOM	1578	0	LYS	81	68.933	22.671	20.696	1.00 28.58	CPS2
ATOM	1579	N	ASP	82	67.487	24.391	20.837	1.00 27.27	CPS2
ATOM	1580	CA	ASP	82	67.741	24.576	22.258	1.00 29.97	CPS2
ATOM	1581	CB	ASP	82	67.521	26.039	22.666	1.00 28.54	CPS2
ATOM	1582	CG	ASP	82	66.074	26.488	22.541	1.00 30.11	CPS2
	1583		ASP	82	65.846	27.715	22.575	1.00 28.52	CPS2
ATOM	1584		ASP	82	65.170	25.633	22.424	1.00 30.87	CPS2
ATOM	1585	С	ASP	82	66.887	23.619	23.095	1.00 30.91	CPS2
ATOM	1586	0	ASP	82	66.268	22.707	22.546	1.00 30.68	CPS2
ATOM	1587	N	GLN	83	66.867	23.819	24.411	1.00 33.59	CPS2
ATOM	1588	CA	GLN	83	66.120	22.941	25.313	1.00 36.28	CPS2
ATOM	1589	CB	GLN	83	66.334	23.356	26.772	1.00 37.73	CPS2
ATOM	1590	CG	GLN	83	65.575	24.608	27.198	1.00 41.41	CPS2
ATOM	1591	CD	GLN	83	66.435	25.862	27.228	1.00 43.65	CPS2
ATOM	1592		GLN	83	66.892	26.355	26.187	1.00 44.27	CPS2
ATOM	1593		GLN	83	66.659	26.389	28.432	1.00 43.27	CPS2
ATOM	1594	С	GLN	83	64.626	22.892	25.022	1.00 37.29	CPS2
ATOM	1595	0	GLN	83	63.943	21.933	25.398	1.00 38.48	CPS2
				-		_ =		2.30 30.40	CF32



MOTA

1652 N CYS 91

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SEP 0 9 2002 **TECH CENTER 1600/2900**

FIG. 1A-28

ATOM 1596 N ASN 24.362 1.00 36.62 84 64.120 23.927 CPS2 ATOM 1597 CA ASN 84 62.707 23.996 24.024 1.00 36.63 CPS2 ATOM 1598 CB ASN 84 62.168 25.389 24.347 1.00 37.40 CPS2 ATOM 1599 CG ASN 84 62.263 25.716 25.828 1.00 38.82 CPS2 ATOM 1600 ODI ASN 84 61.807 24.945 26.675 1.00 39.51 CPS2 ATOM 1601 ND2 ASN 84 62.856 26.857 26.148 1.00 38.34 CPS2 ATOM 1602 C ASN 84 62.456 23.661 22.556 1.00 36.23 CPS2 ATOM 1603 0 ASN 84 61.345 23.839 22.052 1.00 36.16 CPS2 ATOM 1604 N GLY 85 63.492 23.173 21.879 1.00 34.68 CPS2 ATOM 1605 CA GLY 85 63.370 22.814 20.476 1.00 33.60 CPS2 ATOM 1606 С GLY 85 63.425 23.999 19.523 1.00 32.91 CPS2 ATOM 1607 0 GLY 85 63.210 23.841 18.323 1.00 34.92 CPS2 ATOM 1608 N LYS 86 63.726 25.184 20.041 1.00 31.20 CPS2 ATOM 1609 CA LYS 63.781 26.379 86 19.203 1.00 29.67 CPS2 ATOM 1610 CB LYS 86 63.454 27.605 20.052 1.00 31.80 CPS2 ATOM 1611 CG LYS 86 62.137 27.394 20.790 1.00 34.73 CPS2 ATOM 1612 CD LYS 86 61.614 28.628 21.486 1.00 39.19 CPS2 ATOM 1613 CE LYS 86 60.239 28.331 22.094 1.00 41.01 CPS2 ATOM 1614 ΝŻ LYS 86 59.558 29.559 22.592 1.00 43.57 CPS2 ATOM 1615 C LYS 86 65.144 26.492 18.541 1.00 28.23 CPS2 ATOM 1616 0 LYS 86 66.169 26.212 19.159 1.00 27.95 CPS2 ATOM 1617 N PRO 87 65.173 26.922 17.272 1.00 27.01 CPS2 MOTA 1618 CD PRO 87 64.035 27.381 16.447 1.00 26.75 CPS2 ATOM 1619 CA PRO 87 66.427 27.050 16.534 1.00 25.49 CPS2 ATOM 1620 CB PRO 87 65.951 27.164 15.085 1.00 25.44 CPS2 ATOM 1621 CG PRO 27 64.735 28.043 15.239 1.00 27.74 CPS2 ATOM 1622 С PRO 87 67.379 28.185 16.881 1.00 24.72 CPS 2 ATOM 1623 0 PRO 87 66.979 29.270 17.306 1.00 23.36 CPS2 ATOM 1624 N TYP 22 68.664 27.904 16.716 1.00 22.58 CPS2 ATOM 1625 CA TYR 88 69.685 28.924 16.879 1.00 22.24 CPS2 ATOM 1626 CB TYR 88 70.208 29.052 18.324 1.00 22.46 CPS2 ATOM 1627 CG TYP 88 70.921 27.860 18.913 1.00 21.40 CPS2 ATOM 1628 CD1 TYR 88 70.213 26.859 19.577 1.00 21.74 CPS2 ATOM 1629 CE1 TYR 88 70.881 25.796 20.194 1.00 21.69 CPS2 ATOM 1630 CD2 TYR 88 72.317 27.769 18.871 1.00 21.96 CPS2 ATOM 1631 CE2 TYR 88 72.989 26.708 19.480 1.00 20.78 CPS2 ATOM 1632 CZTYR 88 72.262 25.731 20.141 1.00 21.27 CPS2 ATOM 1633 ОН TYR 88 72.923 24.699 20.772 1.00 20.50 CPS2 ATOM 1634 C TYR 88 70.781 28.522 15.912 1.00 22.02 CPS2 ATOM 1635 0 TYP 88 70.897 27.352 15.550 1.00 23.05 CPS2 ATOM 1636 N ILE 89 71.577 29.485 15.480 1.00 21.04 CPS2 ATOM 1637 CA ILE 89 72.623 29.198 14.524 1.00 21.06 CPS2 ATOM 1638 CB 72.573 30.209 TLE 89 13.369 1.00 21.84 CPS2 ATOM 1639 CG2 ILE 89 73.842 30.099 12.513 1.00 22.28 CPS2 ATOM 1640 CG1 ILE 89 71.324 29.982 12.522 1.00 22.51 CPS2 ATOM 1641 CD1 ILE 89 71.172 31.035 11.407 1.00 23.39 CPS2 ATOM 1642 C ILE 89 74.043 29.228 15.072 1.00 22.40 CPS2 ATOM 1643 0 ILE 89 74.401 30.123 15.847 1.00 21.51 CPS2 ATOM 1644 N ILE 90 74.839 28.248 14.644 1.00 21.66 CPS2 ATOM 1645 CA ILE 90 76.255 28.184 14.988 1.00 21.61 CPS2 ATOM 1646 CB ILE 90 76.641 26.878 15.727 1.00 21.37 CPS2 ATOM 1647 CG2 ILE 90 78.169 26.743 15.791 1.00 22.23 CPS2 ATOM 1648 CG1 ILE 90 76.032 26.875 17.134 1.00 20.39 CPS2 ATOM 1649 CD1 ILE 90 76.542 27.991 18.041 1.00 20.47 CPS2 ATOM 1650 С ILE 90 77.019 28.232 13.664 1.00 22.97 CPS2 MOTA 1651 0 ILE 90 76.763 27.437

12.742 1.00 22.67

77.922 29.195 13.559 1.00 23.95

CPS2

CPS2



SEP 0 9 2002

FIG. 1A-29



ATOM	1653	CA	CYS	91	78.769	29.344	12.384	1.00 26.82	CPS2
ATOM	1654	CB	CYS	91	78.229	30.414	11.432	1.00 26.17	CPS2
ATOM	1655	SG	CYS	91	79.260	30.612	9.945	1.00 27.83	CPS2
ATOM	1656	С	CYS	91	80.139	29.760	12.912	1.00 29.07	CPS2
ATOM	1657	0	CYS	91	80.392	30.933	13.149	1.00 29.81	CPS2
ATOM	1658	N	THR	92	81.011	28.784	13.114	1.00 33.43	CPS2
ATOM	1659	CA	THR	92	82.347	29.049	13.637	1.00 37.11	CPS2
ATOM	1660	CB	THR	92	83.080	27.726	13.883	1.00 38.23	CPS2
ATOM	1661		THR	92	82.422	27.027	14.947		
ATOM	1662	CG2	THR	92	84.536	27.971	14.260	1.00 38.10 1.00 40.35	CPS2
ATOM	1663	c	THR	92	83.172	29.947	12.719		CPS2
ATOM	1664	0	THR	92	84.071	30.663		1.00 39.54	CPS2
ATOM	1665	N	LYS	93	82.846	29.916	13.177	1.00 40.49	CPS2
ATOM	1666	CA	LYS	93	83.536		11.432	1.00 40.59	CPS2
ATOM	1667	CB	LYS	93		30.712	10.428	1.00 44.01	CPS2
ATOM	1668	CG	LYS	93	83.024 83.944	30.334	9.040	1.00 45.12	CPS2
ATOM		CD				30.689	7.889	1.00 47.31	CPS2
ATOM	1669 1670		LYS	93	83.519	29.921	6.650	1.00 47.58	CPS2
		CE	LYS	93	84.638	29.817	5.630	1.00 48.24	CPS2
ATOM	1671	NZ	LYS	93	84.290	28.834	4.556	1.00 48.73	CPS2
ATOM	1672	C	LYS	93	83.269	32.183	10.690	1.00 44.95	CPS2
ATOM	1673	0	LYS	93	83.901	33.063	10.112	1.00 46.05	CPS2
ATOM	1674	N	LEU	94	82.322	32.443	11.575	1.00 45.51	CPS2
ATOM	1675	CA	LEU	94	81.964	33.803	11.910	1.00 46.37	CPS2
ATOM	1676	CB	LEU	94	80.452	33.898	12.120	1.00 46.46	CPS2
ATOM	1677	CG	LEU	94	79.830	35.271	12.344	1.00 46.35	CPS2
ATOM	1678		LEU	94	80.037	36.148	11.121	1.00 47.12	CPS2
ATOM	1679	CD2	LEU	94	78.352	35.094	12.615	1.00 46.47	CPS2
ATOM	1680	С	LEU	94	82.685	34.233	13.172	1.00 47.39	CPS2
ATOM	1681	0	LEU	94	82.690	33.511	14.173	1.00 47.30	CPS2
ATOM	1682	N	SER	95	83.319	35.401	13.116	1.00 48.63	CPS2
ATOM	1683	CA	SER	95	84.015	35.941	14.278	1.00 48.81	CPS2
ATOM	1684	CB	SER	95	84.347	37.420	14.037	1.00 49.86	CPS2
ATOM	1685	OG	SER	95	83.229	38.121	13.511	1.00 51.01	CPS2
ATOM	1686	С	SER	95	83.038	35.771	15.448	1.00 48.31	CPS2
ATOM	1687	0	SER	95	81.843	35.585	15.221	1.00 48.26	CPS2
ATOM	1688	N	PRO	96	83.524	35.840	16.704	1.00 45.89	CPS2
ATOM	1689	CD	PRO	96	84.845	36.379	17.068	1.00 46.79	CPS2
ATOM	1690	CA	PRO	96	82.693	35.682	17.909	1.00 45.46	
ATOM	1691	CB	PRO	96	83.678	35.966	19.040	1.00 45.46	CPS2
ATOM	1692	CG	PRO	96	84.573	36.988			CPS2
ATOM	1693	c	PRO	96	81.431	36.544	18.434	1.00 45.85	CPS2
ATOM	1694	ō	PRO	96	81.041		18.033	1.00 44.28	CPS2
ATOM	1695	N	ALA	97		36.911	19.141	1.00 45.08	CPS2
ATOM	1696	CA	ALA	97	80.782	36.839	16.913	1.00 41.71	CPS2
ATOM	1697	CB	ALA		79.577	37.671	16.900	1.00 38.60	CPS2
ATOM	1698			97	79.384	38.246	15.507	1.00 39.14	CPS2
ATOM	1699	0	ALA	97	78.288	36.977	17.347	1.00 36.55	CPS2
ATOM			ALA	97	78.208	35.752	17.405	1.00 36.57	CPS2
	1700	N	ALA	98	77.274	37.784	17.651	1.00 33.65	CPS2
ATOM	1701	CA	ALA	98	75.973	37.270	18.065	1.00 30.93	CPS2
ATOM	1702	CB	ALA	98	75.295	38.239	19.026	1.00 29.97	CPS2
ATOM	1703	C	ALA	98	75.125	37.106	16.804	1.00 28.95	CPS2
ATOM	1704	0	ALA	98	75.077	37.990	15.949	1.00 28.62	CPS2
ATOM	1705	N	VAL	99	74.454	35.969	16.709	1.00 26.50	CPS2
ATOM	1706	CA	VAL	99	73.616	35.659	15.566	1.00 23.47	CPS2
ATOM	1707	CB	VAL	99	74.179	34.437	14.806	1.00 23.08	CPS2
ATOM	1708	CG1		99	73.323	34.125	13.590	1.00 23.46	CPS2
ATOM	1709	CG2	VAL	99	75.617	34.718	14.381	1.00 24.82	CPS2



SEP 0 9 2002

FIG. 1A-30

TECH CENTER 1600/2900

APPROVES | O.G. FIG.

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ATOM	1710	C	VAL	99	72.209	35.335	16.054	1.00 22.87	CPS2
ATOM	1711	0	VAL	99	72.034	34.549	16.980	1.00 23.69	CPS2
ATOM	1712	И	HIS	100	71.208	35.941	15.430	1.00 21.88	CPS2
ATOM	1713	CA	HIS	100	69.819	35.685	15.800	1.00 20.93	CPS2
ATOM	1714	CB	HIS	100	69.152	36.987	16.248	1.00 22.65	CPS2
ATOM	1715	CG	HIS	100	69.930	37.726	17.296	1.00 24.71	CPS2
ATOM	1716		HIS	100	70.837	38.727	17.191	1.00 26.85	CPS2
ATOM	1717	NDI	. HIS	100	69.841	37.430	18.639	1.00 26.27	CPS2
ATOM	1718	CE1	HIS	100	70.658	38.217	19.318	1.00 28.01	CPS2
MOTA	1719	NE2	HIS	100	71.276	39.012	18.462	1.00 25.52	CPS2
ATOM	1720	С	HIS	100	69.124	35.150	14.553	1.00 19.66	CPS2
ATOM	1721	0	HIS	100	69.414	35.596	13.445	1.00 19.28	CPS2
ATOM	1722	N	VAL	101	68.208	34.203	14.729	1.00 20.06	CPS2
MOTA	1723	CA	VAL	101	67.500	33.628	13.586	1.00 18.60	CPS2
ATOM	1724	CB	VAL	101	68.111	32.251	13.166	1.00 18.24	CPS2
ATOM	1725	CG1	VAL	101	67.973	31.236	14.313	1.00 19.48	CPS2
ATOM	1726	CG2	VAL	101	67.436	31.719	11.884	1.00 16.59	CPS2
MOTA	1727	C	VAL	101	66.053	33.403	13.982	1.00 19.22	CPS2
ATOM	1728	0	VAL	101	65.753	33.247	15.160	1.00 20.38	CPS2
ATOM	1729	N	SER	102	65.155	33.451	13.001	1.00 18.44	
ATOM	1730	CA	SER	102	63.748	33.140	13.241	1.00 18.74	CPS2
ATOM	1731	CB	SER	102	62.900	34.393	13.455	1.00 18.74	CPS2
ATOM	1732	OG	SER	102	61.588	33.984	13.804	1.00 18.34	CPS2
ATOM	1733	C	SER	102	63.270	32.398	12.006	1.00 18.22	CPS2
ATOM	1734	0	SER	102	63.568	32.801	10.883	1.00 18.15	CPS2
ATOM	1735	N	ILE	103	62.552	31.300	12.207	1.00 18.21	CPS2
ATOM	1736	CA	ILE	103	62.054	30.511	11.079	1.00 18.76	CPS2
MOTA	1737	CB	ILE	103	62.653	29.079	11.109	1.00 18.76	CPS2
ATOM	1738	CG2	ILE	103	62.224	28.298	9.869	1.00 21.39	CPS2
ATOM	1739	CG1	ILE	103	64.184	29.155	11.156	1.00 21.33	CPS2
ATOM	1740	CD1	ILE	103	64.862	27.789	11.269	1.00 19.93	CPS2
ATOM	1741	С	ILE	103	60.537	30.418	11.198	1.00 21.07	CPS2
ATOM	1742	0	ILE	103	60.004	30.291	12.307	1.00 19.92	CPS2
ATOM	1743	N	THR	104	59.840	30.486	10.066	1.00 19.86	CPS2
ATOM	1744	CA	THR	104	58.388	30.396	10.077		CPS2
MOTA	1745	CB	THR	104	57.743	31.799	9.944	1.00 19.62 1.00 21.91	CPS2
ATOM	1746	OG1	THR	104	56.323	31.708	10.159		CPS2
ATOM	1747		THR	104	58.018	32.390	8.573	1.00 22.12	CPS2
ATOM	1748	С	THR	104	57.945	29.487	8.934	1.00 20.48	CPS2
ATOM	1749	0	THR	104	58.722	29.210	8.016	1.00 20.91	CPS2
ATOM	1750	N	HIS	105	56.705	29.015	8.999	1.00 18.89	CPS2
ATOM	1751	CA	HIS	105	56.179	28.108	7.973	1.00 20.52	CPS2
ATOM	1752	CB	HIS	105	56.224	26.647	8.474	1.00 24.14	CPS2
ATOM	1753	CG	HIS	105	57.594	26.134	8.811	1.00 27.48	CPS2
ATOM	1754	CD2	HIS	105	58.267	26.095	9.987	1.00 32.26	CPS2
ATOM	1755	ND1		105	58.428	25.559	7.874	1.00 33.69	CPS2
ATOM	1756	CE1	HIS	105	59.555	25.191		1.00 34.33	CPS2
ATOM	1757	NE2		105	59.484	25.504	8.457 9.738	1.00 33.58	CPS2
MOTA	1758	С	HIS	105	54.702	28.393		1.00 34.93	CPS2
ATOM	1759	0	HIS	105	53.974	28.944	7.653 8.476	1.00 23.87	CPS2
ATOM	1760	N	THR	106	54.284	28.944		1.00 23.81	CPS2
ATOM	1761	CA	THR	106	52.875		6.449	1.00 23.91	CPS2
ATOM	1762	CB	THR	106	52.484	28.065	6.054	1.00 24.84	CPS2
ATOM	1763	0 G 1		106	53.116	29.199	5.058	1.00 24.13	CPS2
ATOM	1764		THR	106	52.841	28.984	3.792	1.00 25.72	CPS2
ATOM	1765	C	THR	106	52.841	30.571	5.616	1.00 24.87	CPS2
ATOM	1766	ō	THR	106		26.722	5.339	1.00 26.22	CPS2
				100	53.716	25.971	5.224	1.00 25.93	CPS2



SEP 0 9 2002

FIG. 1A-31

TECH CENTER 1600/2900

APPROVED U.G. FIG.
by GLASS SUBCLASS

ATOM	1767	N	LYS	107	51.544	26.408	4.857	1.00 27.42	CPS2
ATOM	1768	CA	LYS	107	51.355	25.135	4.177	1.00 29.72	CPS2
ATOM	1769	CB	LYS	107	49.913	25.013	3.676	1.00 32.60	CPS2
ATOM	1770	CG	LYS	107	49.554	23.612	3.186	1.00 36.45	CPS2
ATOM	1771	CD	LYS	107	48.151	23.568	2.586	1.00 39.60	CPS2
ATOM	1772	CE	LYS	107	48.079	24.346	1.277	1.00 42.78	CPS2
ATOM	1773	NZ	LYS	107	46.750	24.224	0.594	1.00 44.82	CPS2
ATOM	1774	С	LYS	107	52.319	24.941	3.003	1.00 28.95	CPS2
ATOM	1775	0	LYS	107	52.889	23.863	2.833	1.00 29.55	CPS2
ATOM	1776	N	GLU	108	52.524	25.993	2.216	1.00 27.06	CPS2
ATOM	1777	CA	GLU	108	53.374	25.916	1.033	1.00 27.06	CPS2
ATOM	1778	CB	GLU	108	52.639	26.548	-0.155	1.00 29.33	CPS2
ATOM	1779	CG	GLU	108	51.301	25.907	-0.494	1.00 36.04	CPS2
ATOM	1780	CD	GLU	108	51.394	24.407	-0.723	1.00 39.96	CPS2
ATOM	1781	OE1	GLU	108	52.416	23.935	-1.270	1.00 43.61	CPS2
ATOM	1782	OE2	GLU	108	50.430	23.694	-0.370	1.00 43.92	CPS2
ATOM	1783	С	GLU	108	54.771	26.532	1.092	1.00 25.54	CPS2
ATOM	1784	0	GLU	108	55.581	26.311	0.180	1.00 25.56	CPS2
ATOM	1785	N	TYR	109	55.055	27.305	2.138	1.00 24.09	CPS2
ATOM	1786	CA	TYR	109	56.350	27.982	2.250	1.00 21.97	CPS2
ATOM	1787	СВ	TYR	109	56.175	29.480	2.012	1.00 23.30	CPS2
ATOM	1788	CG	TYR	109	55.611	29.823	0.664	1.00 24.68	CPS2
ATOM	1789		TYR	109	56.427	29.842	-0.467	1.00 24.47	CPS2
ATOM	1790		TYR	109	55.895	30.083	-1.731	1.00 25.63	CPS2
ATOM	1791		TYR	109	54.248	30.062	0.505	1.00 25.42	CPS2
ATOM	1792		TYR	109	53.704	30.303	-0.761	1.00 26.80	CPS2
ATOM	1793	cz	TYR	109	54.530	30.307	-1.866	1.00 25.17	CPS2
ATOM	1794	ОН	TYR	109	53.996	30.501	-3.118	1.00 28.15	CPS2
ATOM	1795	c.	TYR	109	57.069	27.849	3.578	1.00 21.24	CPS2
ATOM	1796	ō	TYR	109	56.465	27.578	4.616	1.00 20.80	CPS2
ATOM	1797	N	ALA	110	58.379	28.067	3.518	1.00 21.00	CPS2
ATOM	1798	CA	ALA	110	59.230	28.102	4.705	1.00 21.72	CPS2
ATOM	1799	CB	ALA	110	60.238	26.966	4.686	1.00 22.11	CPS2
ATOM	1800	c	ALA	110	59.945	29.450	4.560	1.00 21.05	CPS2
ATOM	1801	ō	ALA	110	60.301	29.852	3.451	1.00 20.79	CPS2
ATOM	1802	N	ALA	111	60.141	30.165	5.657	1.00 20.04	CPS2
ATOM	1803	CA	ALA	111	60.822	31.446	5.557	1.00 18.91	CPS2
ATOM	1804	CB	ALA	111	59.802	32.577	5.431	1.00 18.42	CPS2
ATOM	1805	C	ALA	111	61.683	31.648	6.785	1.00 17.86	CPS2
ATOM	1806	0	ALA	111	61.400	31.111	7.847	1.00 17.88	CPS2
ATOM	1807	N	ALA	112	62.754	32.411	6.638	1.00 17.82	CPS2
ATOM	1808	CA	ALA	112	63.627	32.642	7.777	1.00 17.98	CPS2
ATOM	1809	CB	ALA	112	64.718	31.564	7.820	1.00 17.38	CPS2
ATOM	1810	C	ALA	112	64.278	33.992		1.00 13.37	CPS2
ATOM	1811	0	ALA	112	64.414	34.527	7.650 6.543	1.00 17.80	CPS2
ATOM	1812	N	GLN	113	64.686	34.540	8.787	1.00 17.80	CPS2
ATOM	1813	CA	GLN	113					
ATOM	1814	CB	GLN	113	65.406	35.802	8.775	1.00 19.02 1.00 21.92	CPS2 CPS2
ATOM	1815	CG	GLN		64.511	36.964	9.178		
ATOM	1816	CD	GLN	113 113	64.045	36.908	10.593	1.00 24.71	CPS2
ATOM	1817		GLN		63.223	38.120	10.979	1.00 27.15	
ATOM	1818			113	62.785	38.239	12.117	1.00 29.66	CPS2
ATOM	1818		GLN	113	63.001	39.019	10.028	1.00 31.94	CPS2
ATOM		С	GLN	113	66.554	35.662	9.764	1.00 18.49	CPS2
	1820	0	GLN	113	66.463	34.908	10.738	1.00 18.27	CPS2
ATOM	1821	N	VAL	114	67.626	36.395	9.506	1.00 18.07	CPS2
ATOM ATOM	1822	CA	VAL	114	68.811	36.355	10.358	1.00 18.90	CPS2
ATOM	1823	CB	VAL	114	69.939	35.488	9.698	1.00 19.24	CPS2



SEP 0 9 2002

FIG. 1A-32

TECH CENTER 1600/2900

APPROVED C.C. F1G.

EV CLASS SUBCLASS
DRAFTSHAN.

ATOM ATOM ATOM ATOM	1824 1825	CG1 CG2		114 114	71.288	35.715	10.406 9.753	1.00 20.55	CPS2
ATOM		CG2	VAL	114			0 752	1 00 20 65	
				114	69.575	34.007	5.755	1.00 20.65	CPS 2
MOTOR	1826	C	VAL	114	69.369	37.757	10.551	1.00 18.95	CPS2
AION	1827	0	VAL	114	69.283	38.595	9.653	1.00 18.70	CPS2
ATOM	1828	N	VAL	115	69.918	38.015	11.733	1.00 18.92	CPS2
ATOM	1829	CA	VAL	115	70.580	39.291	11.989	1.00 19.34	CPS2
ATOM	1830	CB	VAL	115	69.805	40.208	12.970	1.00 19.17	CPS2
ATOM	1831	CG1	VAL	115	70.668	41.445	13.298	1.00 20.91	CPS2
ATOM	1832	CG2	VAL	115	68.499	40.688	12.334	1.00 18.48	CPS2
ATOM	1833	С	VAL	115	71.915	38.927	12.633	1.00 21.35	CPS2
ATOM	1834	0	VAL	115	71.949	38.164	13.590	1.00 21.11	CPS2
ATOM	1835	N	ILE	116	73.009	39.428	12.074	1.00 22.97	CPS2
ATOM	1836	CA	ILE	116	74.333	39.174	12.641	1.00 25.35	CPS2
MOTA	1837	CB	ILE	116	75.359	38.779	11.554	1.00 24.57	CPS2
ATOM	1838	CG2	ILE	116	76.752	38.641	12.177	1.00 25.34	CPS2
ATOM	1839	CG1	ILE	116	74.945	37.468	10.880	1.00 23.64	CPS2
ATOM	1840	CD1	ILE	116	75.862	37.065	9.734	1.00 24.45	CPS2
MOTA	1841	C	ILE	116	74.763	40.511	13.243	1.00 27.82	CPS2
MOTA	1842	0	ILE	116	74.692	41.531	12.569	1.00 26.14	CPS2
ATOM	1843	N	GLU	117	75.176	40.508	14.508	1.00 31.83	CPS2
MOTA	1844	CA	GLU	117	75.620	41.741	15.162	1.00 38.95	CPS2
MOTA	1845	CB	GLU	117	75.075	41.848	16.583	1.00 40.48	CPS2
MOTA	1846	CG	GLU	117	73.585	41.670	16.763	1.00 42.57	CPS2
ATOM.	1847	CD	GLU	117	73.180	41.900	18.211	1.00 43.48	CPS2
ATOM	1848	OE1	GLU	117	73.040	43.075	18.613	1.00 45.02	CPS2
MOTA	1849	OE2	GLU	117	73.029	40.909	18.956	1.00 43.86	CPS2
MOTA	1850	С	GLU	117	77.140	41.701	15.260	1.00 42.69	CPS2
ATOM	1851	0	GLU	117	77.707	40.665	15.598	1.00 44.02	CPS2
ATOM	1852	N	ARG	118	77.803	42.820	14.989	1.00 46.91	CPS2
ATOM	1853	CA	ARG	118	79.259	42.843	15.069	1.00 50.26	'CPS2
ATOM	1854	CB	ARG	118	79.824	43.901	14.124	1.00 52.17	CPS2
MOTA	1855	CG	ARG	118	79.547	45.337	14.529	1.00 54.69	CPS2
MOTA	1856	CD	ARG	118	79.478	46.208	13.288	1.00 57.22	CPS2
ATOM	1857	NE	ARG	118	80.501	45.827	12.319	1.00 59.20	CPS2
ATOM	1858	CZ	ARG	118	80.479	46.170	11.034	1.00 60.31	CPS2
ATOM	1859	NH1	ARG	118	79.483	46.906	10.556	1.00 60.38	CPS2
ATOM	1860	NH2	ARG	118	81.451	45.769	10.224	1.00 60.45	CPS2
ATOM	1861	С	ARG	118	79.722	43.108	16.499	1.00 51.12	CPS2
ATOM	1862	OT1	ARG	118	78.849	43.285	17.380	1.00 51.54	CPS2
ATOM	1863	OT2	ARG	118	80.952	43.125	16.721	1.00 52.39	CPS2
ATOM	1864	С	GLY	1	70.826	44.611	21.183	1.00 31.20	CPS3
ATOM	1865	0	GLY	1	69.832	44.954	21.818	1.00 30.54	CPS3
ATOM	1866	N	GLY	1	72.197	46.046	22.695	1.00 34.55	CPS3
ATOM	1867	CA	GLY	1	72.168	45.285	21.411	1.00 32.26	CPS3
ATOM	1868	N	ILE	2	70.797	43.643	20.274	1.00 29.14	CPS3
ATOM	1869	CA	ILE	2	69.562	42.935	19.973	1.00 27.23	CPS3
ATOM	1870	CB	ILE	2	69.544	42.452	18.510	1.00 28.42	CPS3
ATOM	1871	CG2	ILE	2	68.334	41.538	18.271	1.00 29.40	CPS3
ATOM	1872	CG1	ILE	2	69.495	43.670	17.576	1.00 28.86	CPS3
ATOM	1873	CD1	ILE	2	69.507	43.331	16.115	1.00 31.24	CPS3
ATOM	1874	С	ILE	2	69.332	41.748	20.883	1.00 26.26	CPS3
ATOM	1875	0	ILE	2	70.213	40.893	21.040	1.00 25.80	CPS3
ATOM	1876	N	TYR	3	68.147	41.713	21.489	1.00 24.05	CPS 3
ATOM	1877	CA	TYR	3	67.752	40.622	22.369	1.00 24.41	CPS
ATOM	1878	CB	TYR	3	66.682	41.080	23.352	1.00 26.14	CPS3
MOTA	1879	CG	TYR	3	66.254	39.967	24.268	1.00 28.89	CPS3
ATOM	1880		TYR	3	67.098	39.514	25.290	1.00 29.65	CPS3





SEP 0 9 2002

TECH CENTER 1600/2900

	SUBCLASS	٦
0.6. FIG.	FLASS SUBC	
APPROVED	5	DRAFTSHAM

ATOM	1881		TYR	3	66.736	38.442	26.092	1.00 32.21	CPS3
ATOM	1882		TYR	3	65.037	39.316	24.080	1.00 29.35	CPS3
ATOM	1883		TYR	3	64.667	38.235	24.883	1.00 31.35	CPS3
ATOM	1884	CZ	TYR	3	65.520	37.806	25.881	1.00 32.89	CPS3
MOTA	1885	OH	TYR	3	65.160	36.730	26.660	1.00 35.01	CPS3
MOTA	1886	C	TYR	3	67.190	39.454	21.551	1.00 23.32	CPS3
ATOM	1887	0	TYR	3	67.604	38.305	21.720	1.00 22.34	CPS3
ATOM	1888	N	GLY	4	66.240	39.75 5	20.667	1.00 21.28	CPS3
ATOM	1889	CA	GLY	4	65.655	38.705	19.848	1.00 20.37	CPS3
MOTA	1890	C	GLY	4	64.945	39.231	18.614	1.00 18.42	CPS3
ATOM	1891	0	GLY	4	64.636	40.411	18.527	1.00 18.04	CPS3
ATOM	1892	N	ILE	5	64.694	38.350	17.656	1.00 17.82	CPS3
ATOM	1893	CA	ILE	5	63.990	38.736	16.432	1.00 17.02	CPS3
ATOM	1894	CB	ILE	5	64.939	38.802	15.206	1.00 16.53	CPS3
ATOM	1895		ILE	5	66.110	39.753	15.514	1.00 17.11	CPS3
ATOM	1896		ILE	5	65.457	37.398	14.841	1.00 16.93	CPS3
ATOM	1897		ILE	5	66.404	37.390	13.622	1.00 18.91	CPS3
ATOM	1898	C	ILE	5	62.932	37.669	16.202	1.00 17.16	CPS3
ATOM	1899	0	ILE	5	63.033	36.555	16.737	1.00 16.49	CPS3
ATOM	1900	N	GLY	6	61.900	38.010	15.441	1.00 16.65	CPS3
ATOM	1901	CA	GLY	6	60.847	37.041	15.187	1.00 17.04	CPS3
ATOM	1902	C	GLY	6	60.217	37.338	13.844	1.00 17.86	CPS3
MOTA	1903	0	GLY	6	60.070	38.500	13.472	1.00 16.46	CPS3
ATOM	1904	N	LEU	7	59.865	36.283	13.110	1.00 18.17	CPS3
ATO:	1905	CA	LEU	7	59.257	36.432	11.795	1.00 18.15	CPS3
ATOM	1906	CB	LEU	7	60.258	36.047	10.698	1.00 17.40	CPS3
ATOM	1907	CG	LEU	7	59.723	35.991	9.257	1.00 17.71	CPS3
ATOM	1908		LEU	7	59.370	37.420	8.785	1.00 18.00	CPS3
ATOM	1909		LEU	7	60.775	35.357	8.330	1.00 18.26	CPS3
ATOM	1910	C	LEU	7	58.068	35.482	11.718	1.00 18.31	CPS3
ATOM	1911	0	LEU	7	58.121	34.371	12.236	1.00 18.61	CPS3
ATOM	1912	N	ASP	8	56.992	35.923	11.083	1.00 18.46	CPS3
ATOM	1913	CA	ASP	8	55.849	35.043	10.911	1.00 18.86	CPS3
ATOM	1914	CB	ASP	8	54.871	35.157	12.082	1.00 19.63	CPS 3
ATOM	1915	CG	ASP	8	53.642	34.294	11.881	1.00 22.43	CPS3
ATOM	1916		ASP	8	52.653	34.768	11.281	1.00 23.32	CPS3
ATOM	1917	OD2		8	53.683	33.126	12.294	1.00 24.61	CPS3
	1918	С	ASP	8	55.107	35.350	9.632	1.00 19.01	CPS3
MOTA	1919	0	ASP	8	54.955	36.507	9.251	1.00 19.92	CPS3
ATOM	1920	N	ILE	9	54.671	34.302	8.946	1.00 18.64	CPS3
ATOM ATOM	1921	CA	ILE	9	53.871	34.490	7.747	1.00 20.14	CPS3
ATOM	1922	CB	ILE	9	54. 5 65	33.982	6.468	1.00 19.98	CPS3
ATOM	1923	CG2		9	53.605	34.144	5.283	1.00 20.49	CPS3
ATOM	1924	CG1		9	55.843	34.782	6.213	1.00 20.86	CPS3
ATOM	1925	CD1		9	56.635	34.318	4.987	1.00 23.49	CPS3
ATOM	1926	C	ILE	9	52.642	33.649	8.032	1.00 20.08	CPS3
ATOM	1927	0	ILE	9	52.760	32.500	8.472	1.00 21.18	CPS3
ATOM	1928	N	THR	10	51.470	34.224	7.793	1.00 20.82	CPS3
ATOM	1929	CA	THR	10	50.218	33.543	8.064	1.00 22.22	CPS3
ATOM	1930	CB	THR	10	49.502	34.213	9.267	1.00 23.80	CPS3
ATOM	1931	OG1		10	50.237	33.942	10.478	1.00 22.74	CPS3
ATOM	1932		THR	10	48.088	33.667	9.413	1.00 24.86	CPS3
ATOM	1933	C	THR	10	49.310	33.548	6.838	1.00 22.47	CPS3
ATOM	1934		THR	10	49.106	34.581	6.197	1.00 22.06	CPS3
ATOM ATOM	1935		GLU	11	48.784	32.377	6.508	1.00 23.62	CPS3
ATOM	1936		GLU	11	47.894	32.230	5.359	1.00 25.07	CPS3
ALON	1937	CB	GLU	11	47.846	30.757	4.940	1.00 25.66	CPS3



SEP 0 9 2002

·16.	SUBCLASS	
0.6. F	UASS	
APPROVED	У6	ORAFTSKAN

ATOM	1938	CG	GLU	11	46.898	30.463	3.793	1.00 29.78	CPS3
MOTA	1939	CD	GLU	11	46.798	28.980	3.481	1.00 32.43	CPS3
ATOM	1940	OE1		11	47.101	28.151	4.373	1.00 34.21	CPS3
ATOM	1941	OE2	GLU	11	46.396	28.643	2.346	1.00 34.51	CPS3
MOTA	1942	C	GLU	11	46.502	32.708	5.771	1.00 25.06	CPS3
ATOM	1943	0	GLU	11	45.922	32.173	6.714	1.00 25.54	CPS3
ATOM	1944	N	LEU	12	45.963	33.701	5.069	1.00 25.35	CPS3
MOTA	1945	CA	LEU	12	44.642	34.234	5.403	1.00 26.43	CPS3
ATOM	1946	CB	LEU	12	44.225	35.329	4.408	1.00 28.34	CPS3
ATOM	1947	CG	LEU	12	44.432	36.787	4.846	1.00 30.12	CPS3
ATOM	1948	CD1	LEU	12	45.896	37.051	5.095	1.00 29.84	CPS3
ATOM	1949	CD2	LEU	12	43.898	37.731	3.771	1.00 31.67	CPS3
ATOM	1950	С	LEU	12	43.552	33.163	5.459	1.00 27.18	CPS3
ATOM	1951	0	LEU	12	42.700	33.183	6.350	1.00 25.07	CPS3
ATOM	1952	1.1	ALA	13	43.585	32.231	4.511	1.00 26.60	CPS3
ATOM	1953	CA	ALA	13	42.602	31.160	4.467	1.00 27.39	CPS3
ATOM	1954	CB	ALA	13	42.836	30.296	3.227	1.00 28.53	CPS3
ATOM	1955	C	ALA	13	42.616	30.293	5.730	1.00 28.85	CPS3
ATOM	1956	0	ALA	13	41.569	29.793	6.158	1.00 29.11	CPS3
ATOM	1957	N	ARG	14	43.790	30.115	6.332	1.00 28.68	CPS3
ATOM	1958	CA	ARG	14	43.898	29.303	7.536	1.00 29.64	CPS3
ATOM	1959	CB	ARG	14	45.361	28.961	7.844	1.00 31.16	CPS3
ATOM	1960	CG	ARG	14	45.520	27.811	8.831	1.00 33.62	CPS3
ATOM	1961	CD	ARG	14	46.961	27.333	8.931	1.00 36.46	CPS3
ATOM	1962	NE	ARG	14	47.813	28.263	9.669	1.00 39.10	CPS3
ATOM	1963	CZ	ARG	14	47.809	28.400	10.993	1.00 39.42	CPS3
ATOM	1964	NH1	ARG	14	46.998	27.665	11.741	1.00 41.04	CPS3
ATOM	1965	NH2	ARG	14	48.618	29.273	11.572	1.00 39.96	CPS3
ATOM	1966	С	ARG	14	43.277	30.067	8.693	1.00 30.10	CPS3
ATOM	1967	0	ARG	14	42.619	29.473	9.549	1.00 30.68	CPS3
MOTA	1968	N	ILE	15	43.490	31.382	8.721	1.00 28.50	CPS3
ATOM	1969	CA	ILE	15	42.904	32.220	9.765	1.00 29.44	CPS3
ATOM	1970	CB	ILE	15	43.322	33.708	9.611	1.00 28.52	CPS3
ATOM	1971	CG2	ILE	15	42.492	34.596	10.544	1.00 27.32	CPS3
ATOM	1972	CG1	ILE	15	44.809	33.865	9.955	1.00 27.87	CPS3
ATOM	1973	CD1	ILE	15	45.145	33.454	11.384	1.00 29.13	CPS3
ATOM	1974	C	ILE	15	41.383	32.116	9.656	1.00 30.89	CPS3
ATOM	1975	0	ILE	15	40.689	31.904	10.654	1.00 31.81	CPS3
MOTA	1976	N	ALA	16	40.868	32.271	8.439	1.00 31.30	CPS3
ATOM	1977	CA	ALA	16	39.427	32.180	8.223	1.00 33.08	CPS3
ATOM	1978	CB	ALA	16	39.096	32.463	6.760	1.00 33.09	CPS3
ATOM	1979	C	ALA	16	38.902	30.802	8.634	1.00 34.30	CPS3
ATOM	1980	0	ALA	16	37.800	30.695	9.169	1.00 35.45	CPS3
ATOM	1981	N	SER	17	39.689	29.753	8.395	1.00 35.66	CPS3
ATOM	1982	CA	SER	17	39.282	28.396	8.764	1.00 38.32	CPS3
ATOM	1983	CB	SER	17	40.271	27.356	8.227	1.00 39.07	CPS3
ATOM	1984	OG	SER	17	40.290	27.332	6.810	1.00 40.78	CPS3
ATOM	1985	С	SER	17	39.187	28.242	10.277	1.00 40.41	CPS3
ATOM	1986	0	SER	17	38.202	27.704	10.789	1.00 40.87	CPS3
ATOM	1987	N	MET	18	40.215	28.704	10.989	1.00 41.04	CPS3
ATOM	1988	CA	MET	18	40.238	28.621	12.449	1.00 42.44	CPS3
ATOM	1989	CB	MET	18	41.582	29.110	13.004	1.00 42.96	CPS3
ATOM	1990	CG	MET	18	42.774	28.251	12.617	1.00 44.33	CPS3
ATOM	1991	SD	MET	18	44.266	28.670	13.558	1.00 48.01	CPS3
ATOM	1992	CE	MET	18	44.718	30.192	12.791	1.00 43.96	CPS3
ATOM	1993	С	MET	18	39.115	29.448	13.055	1.00 42.50	CPS3
ATOM	1994	0	MET	18	38.472	29.026	14.014	1.00 43.21	CPS3
							24.024		



SEP 0 9 2002 TECH CENTER 1600/2900

<u>l</u> G.	SUBCLAS	
0.G.F	01.755	
APPROVED	¥6	DRAFISMAN

MOTA	1995	N	ALA	19	38.886	30.629	12.496	1.00 43.10	CPS3
ATOM	1996	CA	ALA	19	37.838	31.517	12.981	1.00 44.50	CPS3
ATOM	1997	CB	ALA	19	37.901	32.844	12.233	1.00 45.06	CPS3
ATOM	1998	c	ALA	19	36.453	30.889	12.816	1.00 46.48	CPS3
ATOM	1999	ō	ALA	19	35.541	31.155	13.603	1.00 46.54	
ATOM	2000	N	GLY	20	36.296	30.061	11.788		CPS3
ATOM	2001	CA	GLY	20				1.00 47.19	CPS3
					35.015	29.417	11.558	1.00 48.52	CPS3
ATOM	2002	C	GLY	20	34.838	28.190	12.429	1.00 48.97	CPS3
ATOM	2003	0	GLY	20	33.754	27.928	12.945	1.00 49.64	CPS3
ATOM	2004	N	ARG	21	35.921	27.443	12.599	1.00 49.96	CPS3
ATOM	2005	CA	ARG	21	35.915	26.227	13.397	1.00 50.93	CPS3
ATOM	2006	CB	ARG	21	37.083	25.336	12.963	1.00 52.93	CPS3
ATOM	2007	CG	ARG	21	37.367	24.152	13.872	1.00 55.96	CPS3
ATOM	2008	CD	ARG	21	36.136	23.278	14.055	1.00 58.49	CPS3
ATOM	2009	NE	ARG	21	36.396	22.145	14.940	1.00 60.33	CPS3
ATOM	2010	CZ	ARG	21	35.448	21.371	15.457	1.00 60.98	CPS3
MOTA	2011	NH1	ARG	21	34.171	21.611	15.179	1.00 61.06	CPS3
ATOM	2012		ARG	21	35.776	20.356	16.247	1.00 61.52	CPS3
ATOM	2013	С	ARG	21	35.987	26.469	14.904	1.00 51.00	
ATOM	2014	ō	ARG	21	35.437	25.698	15.693	1.00 51.31	CPS3
ATOM	2015	N	GLN	22	36.655	27.543			CPS3
ATOM	2016	CA	GLN	22			15.307	1.00 50.09	CPS3
ATOM	2017	CB	GLN	22	36.807	27.835	16.725	1.00 49.10	CPS3
ATOM					38.224	28.330	17.011	1.00 48.88	CPS3
	2018	CG	GLN	22	39.273	27.241	16.967	1.00 49.46	CPS3
ATOM	2019	CD	GLN	22	40.653	27.759	17.297	1.00 49.87	CPS3
ATOM	2020		GLN	22	40.828	28.529	18.242	1.00 50.04	CPS3
ATOM	2021		GLN	22	41.648	27.330	16.526	1.00 50.52	CPS3
ATOM	2022	C	GLN	22	35.822	28.816	17.328	1.00 47.67	CPS3
ATOM	2023	0	GLN	22	35.309	29.716	16.660	1.00 48.35	CPS3
ATOM	2024	N	LYS	23	35.580	28.626	18.619	1.00 46.19	CPS3
MOTA	2025	CA	LYS	23	34.683	29.477	19.384	1.00 44.06	CPS3
ATOM	2026	CB	LYS	23	34.086	28.701	20.569	1.00 45.41	CPS3
ATOM	2027	CG	LYS	23	34.474	27.218	20.651	1.00 48.30	CPS3
ATOM	2028	CD	LYS	23	35.983	27.019	20.828	1.00 50.15	CPS3
ATOM	2029	CE	LYS	23	36.341	25.554	21.037	1.00 51.50	CPS3
MOTA	2030	NZ	LYS	23	35.720	25.007	22.285	1.00 51.24	CPS3
ATOM	2031	C	LYS	23	35.490	30.659	19.918	1.00 40.79	CPS3
ATOM	2032	0	LYS	23	36.523	30.457	20.558	1.00 40.61	CPS3
ATOM	2033	N	ARG	24	35.029	31.878	19.630	1.00 36.53	CPS3
ATOM	2034	CA	ARG	24	35.671	33.110	20.103	1.00 33.31	CPS3
ATOM	2035	CB	ARG	24	35.675	33.110	21.630		
ATOM	2036	CG	ARG	24	34.367			1.00 32.78	CPS3
ATOM	2037	CD	ARG			32.793	22.310	1.00 34.25	CPS3
ATOM	2038	NE	ARG	24	33.299	33.846	22.126	1.00 35.40	CPS3
ATOM	2038	CZ		24	32.105	33.476	22.883	1.00 38.23	CPS3
ATOM	2040		ARG	24	30.866	33.783	22.520	1.00 38.00	CPS3
		NH1		24	30.653	34.474	21.405	1.00 38.06	CPS3
ATOM	2041		ARG	24	29.841	33.375	23.259	1.00 39.67	CPS3
ATOM	2042	С	ARG	24	37.116	33.301	19.641	1.00 31.71	CPS3
ATOM	2043	0	ARG	24	37.930	33.845	20.393	1.00 27.62	CPS3
ATOM	2044	N	PHE	25	37.441	32.880	18.421	1.00 29.27	CPS3
ATOM	2045	CA	PHE	25	38.816	33.016	17.950	1.00 28.40	CPS3
ATOM	2046	CB	PHE	25	38.958	32.446	16.539	1.00 28.43	CPS3
ATOM	2047	CG	PHE	25	40.370	32.482	16.011	1.00 28.82	CPS3
ATOM	2048	CD1	PHE	25	40.758	33.450	15.097	1.00 29.33	CPS3
ATOM	2049	CD2		25	41.311	31.556	16.445	1.00 30.13	CPS3
ATOM	2050	CE1		25	42.067	33.500	14.618	1.00 30.13	CPS3
ATOM	2051	CE2		25	42.625	31.597	15.970	1.00 30.32	CPS3
				~ 3	42.025	31.33/	15.9/0	1.00 30.21	CPSS



SEP 0 9 2002

TECH CENTER 1600/2900



	SS	
F16.	SUBCLASS	
J.G. F	1.455	
1	12.	SHAK
APPROVE	· 6	DRAFTSHAN

ATOM	2052	CZ	PHE	25	42.997	32.570	15.059	1.00 29.47	CPS3
ATOM	2053	C	PHE	25	39.325	34.455	17.992	1.00 27.06	CPS3
ATOM	2054	0	PHE	25	40.394	34.716	18.531	1.00 27.13	CPS3
ATOM	2055	N	ALA	26	38.569	35.394	17.433	1.00 27.40	CPS3
ATOM	2056	CA	ALA	26	38.996	36.793	17.441	1.00 26.90	CPS3
ATOM	2057	CB	ALA	26	37.987	37.661	16.692	1.00 27.98	CPS3
ATOM	2058	С	ALA	26	39.174	37.302	18.869	1.00 26.90	CPS3
ATOM	2059	0	ALA	26	40.131	38.027	19.170	1.00 25.61	CPS3
ATOM	2060	N	GLU	27	38.254	36.912	19.753	1.00 25.63	CPS3
ATOM	2061	CA	GLU	27	38.314	37.329	21.143	1.00 25.29	CPS3
ATOM	2062	CB	GLU	27	37.070	36.864	21.908	1.00 25.87	CPS3
ATOM	2063	CG	GLU	27	35.815	37.656	21.612	1.00 26.46	CPS3
ATOM	2064	CD	GLU	27	35.199	37.336	20.266	1.00 28.64	CPS3
ATOM	2065		GLU	27	35.569	36.324	19.633	1.00 29.62	CPS3
ATOM	2066		GLU	27	34.319	38.106	19.845	1.00 29.62	CPS3
ATOM	2067	C	GLU	27	39.548	36.770			
ATOM							21.835	1.00 24.48	CPS3
	2068	0	GLU	27	40.026	37.340	22.812	1.00 23.69	CPS3
ATOM	2069	И	ARG	28	40.057	35.652	21.336	1.00 24.10	CPS3
ATOM	2070	CA	ARG	28	41.235	35.046	21.937	1.00 25.35	CPS3
ATOM	2071	CB	ARG	28	41.286	33.561	21.588	1.00 26.74	CPS3
MOTA	2072	CG	ARG	28	42.365	32.796	22.331	1.00 30.57	CPS3
ATOM	2073	CD	ARG	28	42.064	31.303	22.339	1.00 33.01	CPS3
ATOM	2074	NE	ARG	28	42.094	30.724	21.001	1.00 34.13	CPS3
ATOM	2075	CZ	ARG	28	43.212	30.481	20.327	1.00 36.89	CPS3
MOTA	2076		ARG	28	44.389	30.768	20.871	1.00 37.04	CPS3
ATOM	2077		ARG	28	43.157	29.946	19.111	1.00 37.15	CPS3
ATOM	2078	C	ARG	28	42.529	35.736	21.488	1.00 24.56	CPS3
ATOM	2079	0	ARG	28	43.450	35.930	22.282	1.00 24.22	CPS3
ATOM	2080	N	ILE	29	42.574	36.130	20.225	1.00 23.52	CPS3
ATOM	2081	CA	ILE	29	43.760	36.773	19.657	1.00 24.20	CPS3
ATOM	2082	CB	ILE	29	43.788	36.591	18.122	1.00 24.82	CPS3
ATOM	2083	CG2		29	45.074	37.184	17.538	1.00 25.66	CPS3
ATOM	2084		ILE	29	43.627	35.107	17.768	1.00 26.45	CPS3
ATOM	2085	CD1	ILE	29	44.675	34.207	18.357	1.00 26.17	CPS3
ATOM	2086	C	ILE	29	43.866	38.270	19.932	1.00 24.20	CPS3
ATOM	2087	0	ILE	29	44.964	38.795	20.164	1.00 23.59	CPS3
ATOM	2088	N	LEU	30	42.722	38.952	19.913	1.00 22.23	CPS3
ATOM	2089	CA	LEU	30	42.683	40.401	20.076	1.00 22.20	CPS3
ATOM	2090	CB	LEU	30-	41.643	40.977	19.106	1.00 21.52	CPS3
ATOM	2091	CG	LEU	30	41.738	40.518	17.649	1.00 22.01	CPS3
ATOM	2092	CD1	LEU	30	40.591	41.151	16.857	1.00 22.54	CPS3
ATOM	2093	CD2	LEU	30	43.104	40.926	17.051	1.00 22.99	CPS3
ATOM	2094	С	LEU	30	42.387	40.940	21.467	1.00 22.82	CPS3
ATOM	2095	0	LEU	30	41.622	40.342	22.216	1.00 22.70	CPS3
ATOM	2096	N	THR	31	42.995	42.080	21.798	1.00 22.58	CPS3
ATOM	2097	CA	THR	31	42.752	42.741	23.076	1.00 23.08	CPS3
ATOM	2098	CB	THR	31	43.781	43.846	23.374	1.00 22.96	CPS3
ATOM	2099	OG1	THR	31	43.666	44.871	22.377	1.00 23.51	CPS3
ATOM	2100	CG2	THR	31	45.200	43.283	23.406	1.00 23.16	CPS3
ATOM	2101	С	THR	31	41.400	43.438	22.944	1.00 23.05	CPS3
ATOM	2102	ō	THR	31	40.840	43.499	21.850	1.00 20.90	CPS3
ATOM	2103	N	ARG	32	40.887	43.992	24.042	1.00 23.64	CPS3
MOTA	2104	CA	ARG	32	39.593	44.672	23.984	1.00 25.29	CPS3
ATOM	2105	СВ	ARG	32	39.224	45.258	25.346	1.00 24.83	CPS3
ATOM	2106	CG	ARG	32	39.005	44.220	26.419	1.00 24.83	CPS3
ATOM	2107	CD	ARG	32	38.684	44.220		1.00 25.80	CPS3
ATOM	2108	NE	ARG	32	38.513	44.890	27.752	1.00 25.11	CPS3
	0			52	30.313	43.908	28.819	1.00 25.70	CPSS



SEP 0 9 2002

TECH CENTER 1600/2900



FIG.	SUBCLASS	
0.6.	PLASS	
APPROVED	1.2	DRAFTSKAN

ATOM	2109	CZ	ARG	32	38.361	44.218	30.101	1.00 25.97	CPS3
ATOM	2110	NH1	ARG	32	38.357	45.492	30.481	1.00 26.33	CPS3
ATOM	2111	NH2	ARG	32	38.224	43.256	31.005	1.00 27.07	CPS3
ATOM	2112	C	ARG	32	39.570	45.789	22.953	1.00 25.39	CPS3
ATOM	2113	0	ARG	32	38.608	45.912	22.187	1.00 24.58	CPS3
MOTA	2114	N	SER	33	40.622	46.605	22.935	1.00 24.96	CPS3
ATOM	2115	CA	SER	33	40.699	47.715	21.988	1.00 25.69	CPS3
ATOM	2116	CB	SER	33	41.909	48.603	22.284	1.00 27.21	CPS3
MOTA	2117	OG	SER	33	41.714	49.345	23.469	1.00 28.30	CPS3
ATOM	2118	C	SER	33	40.766	47.250	20.544	1.00 25.41	CPS3
ATOM	2119	0	SER	33	40.180	47.870	19.664	1.00 25.68	
MOTA	2120	N	GLU	34	41.492	46.169	20.290	1.00 24.03	CPS3
ATOM	2121	CA	GLU	34	41.597	45.640	18.935	1.00 23.95	CPS3
ATOM	2122	CB	GLU	34	42.699	44.574	18.879	1.00 23.95	CPS3
ATOM	2123	CG	GLU	34	44.089	45.163	19.059		CPS3
ATOM	2124	CD	GLU	34	45.182	44.105		1.00 21.69	CPS3
ATOM	2125	OE1	GLU	34	46.328	44.105	19.221	1.00 22.84	CPS3
ATOM	2126		GLU	34			18.837	1.00 21.34	CPS3
ATOM	2127	C	GLU	34	44.900	42.996	19.740	1.00 20.06	CPS3
ATOM	2128	o	GLU	34		45.051	18.516	1.00 25.26	CPS3
ATOM	2129	N	LEU	35	39.846	45.151	17.353	1.00 25.38	CPS3
ATOM	2130	CA	LEU		39.548	44.433	19.472	1.00 24.79	CPS3
ATOM	2131	CB		35	38.231	43.849	19.211	1.00 25.97	CPS3
ATOM	2132	CG	LEU	35	37.678	43.160	20.462	1.00 27.07	CPS3
MOTA			LEU	35	37.717	41.639	20.630	1.00 30.32	CPS3
ATOM	2133		LEU	35	36.834	41.312	21.844	1.00 30.54	CPS3
ATOM	2134		LEU	35	37.201	40.893	19.391	1.00 28.41	CPS3
	2135	C	LEU	35	37.264	44.947	18.806	1.00 25.13	CPS3
MOTA	2136	0	LEU	35	36.471	44.778	17.885	1.00 26.21	CPS3
ATOM	2137	N	ASP	36	37.310	46.066	19.518	1.00 25.47	CPS3
ATOM	2138	CA	ASP	36	36.432	47.180	19.189	1.00 26.39	CPS3
MOTA	2139	CB	ASP	36	36.696	48.383	20.111	1.00 27.06	CPS3
ATOM	2140	CG	ASP	36	36.203	48.148	21.531	1.00 30.18	CPS3
ATOM	2141	OD1		36	35.336	47.272	21.710	1.00 28.81	CPS3
ATOM	2142	OD2		36	36.667	48.843	22.464	1.00 29.67	CPS3
ATOM	2143	С	ASP	36	36 .6 38	47.580	17.733	1.00 28.21	CPS3
ATOM	2144	0	ASP	36	35.674	47.866	17.024	1.00 27.00	CPS3
ATOM	2145	N	GLN	37	37.892	47.580	17.281	1.00 28.66	CPS3
ATOM	2146	CA	GLN	37	38.200	47.939	15.895	1.00 28.46	CPS3
ATOM	2147	CB	GLN	37	39.712	48.129	15.705	1.00 31.40	CPS3
ATOM	2148	CG	GLN	37	40.309	49.384	16.315	1.00 34.73	CPS3
ATOM	2149	CD	GLN	37	41.820	49.462	16.104	1.00 37.78	CPS3
ATOM	2150		GLN	37	42.601	48.806	16.803	1.00 38.25	CPS3
ATOM	2151	NE2		37	42.233	50.256	15.128	1.00 40.09	CPS3
ATOM	2152	С	GLN	37	37.729	46.838	14.954	1.00 28.42	CPS3
ATOM	2153	0	GLN	37	37.107	47.097	13.918	1.00 28.25	CPS3
ATOM	2154	И	TYR	38	38.040	45.602	15.322	1.00 25.92	CPS3
ATOM	2155	CA	TYR	38	37.676	44.445	14.526	1.00 27.76	CPS3
ATOM	2156	CB	TYR	38	38.124	43.179	15.268	1.00 26.65	CPS3
ATOM	2157	CG	TYR	38	37.674	41.867	14.666	1.00 28.74	CPS3
ATOM	2158	CD1	TYR	38	36.522	41.225	15.130	1.00 27.49	CPS3
ATOM	2159	CE1	TYR	38	36.105	40.013	14.583	1.00 27.49	CPS3
ATOM	2160	CD2		38	38.397	41.264	13.636	1.00 27.76	CPS3
ATOM	2161	CE2		38	37.986	40.046	13.030	1.00 27.76	CPS3
ATOM	2162	CZ	TYR	38	36.840	39.430	13.565	1.00 29.24	CPS3
ATOM	2163	OH	TYR	38	36.440	38.218	13.565	1.00 29.43	CPS3
ATOM	2164	c	TYR	38	36.177	44.398	14.219	1.00 30.36	CPS3
MOTA	2165	ō	TYR	38	35.776				
		-			33.110	44.169	13.075	1.00 28.54	CPS3



TECH CENTER 1600/2900

0.6. FIG.	CLASS SUBCLASS	
APPROVE	1.6	DRAFTSMAN

ATOM 2169 CB TYR 39 33.910 44.575 15.018 1.00 31.58 ATOM 2169 CG TYR 39 33.2839 42.054 16.068 1.00 31.89 ATOM 2171 CEL TYR 39 32.839 42.054 16.068 1.00 31.89 ATOM 2171 CEL TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2171 CEL TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2171 CEL TYR 39 32.839 42.054 16.068 1.00 32.76 ATOM 2173 CEZ TYR 39 33.658 42.808 18.185 1.00 32.76 ATOM 2173 CEZ TYR 39 33.658 42.808 18.185 1.00 32.76 ATOM 2173 CEZ TYR 39 33.658 42.808 18.185 1.00 32.76 ATOM 2175 CE TYR 39 33.339 0.455 17.760 1.00 33.06 ATOM 2175 CE TYR 39 33.309 0.455 17.760 1.00 33.06 ATOM 2175 CE TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2176 CE TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2177 CE TYR 39 33.277 45.627 14.110 1.00 33.88 ATOM 2177 CE GE GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2178 CE GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2180 CE GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2180 CE GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2181 CE GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.374 50.110 13.879 1.00 46.21 ATOM 2180 CE GLU 40 33.388 47.452 11.423 1.00 38.62 ATOM 2185 CE GLU 40 33.515 48.895 15.706 1.00 46.21 ATOM 2180 CE GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2185 CE GLU 40 33.491 48.200 10.530 1.00 39.32 ATOM 2185 CE GLU 41 33.5120 46.028 9.851 1.00 37.52 ATOM 2180 CE GLU 41 33.5120 46.028 9.851 1.00 37.52 ATOM 2180 CE GLU 41 33.520 47.514 10.794 1.00 38.83 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.63 ATOM 2190 CE GLEU 41 37.520 47.514 10.794 1.00 38.											
ATOM 2169 CB TYR 39 33.195 44.515 16.367 1.00 31.24 ATOM 2169 CG TYR 39 33.195 44.515 16.367 1.00 31.24 ATOM 2170 CD1 TYR 39 32.839 42.054 16.068 1.00 31.89 ATOM 2171 CE1 TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2172 CD2 TYR 39 33.658 42.808 18.185 1.00 32.76 ATOM 2173 CE2 TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.739 40.455 17.760 1.00 33.06 ATOM 2175 OH TYR 39 33.739 40.455 17.760 1.00 33.06 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 34.53 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 34.58 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2178 N GLU 40 34.026 46.666 13.766 13.766 1.00 34.54 ATOM 2178 N GLU 40 34.026 46.666 13.766 13.766 1.00 35.41 ATOM 2180 CB GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.555 1.00 44.70 ATOM 2181 CB GLU 40 33.553 49.545 14.556 1.00 34.70 ATOM 2182 CD GLU 40 33.553 49.545 14.556 1.00 44.70 ATOM 2180 CB GLU 40 33.553 49.545 14.556 1.00 44.70 ATOM 2180 CB GLU 40 33.551 49.555 14.755 1.00 44.23 ATOM 2180 CB GLU 40 33.551 49.555 14.755 1.00 44.23 ATOM 2180 CB GLU 40 33.551 49.555 14.755 1.00 44.23 ATOM 2180 CB GLU 40 33.551 49.555 14.755 1.00 39.04 ATOM 2180 CB GLU 40 33.551 49.555 14.755 1.00 39.31 ATOM 2185 C GLU 40 33.881 47.452 11.423 10.00 38.62 ATOM 2185 C GLU 40 33.881 47.452 11.423 10.00 38.62 ATOM 2185 C GLU 40 33.881 47.452 11.423 10.00 38.62 ATOM 2185 C GLU 40 33.881 47.452 11.423 10.00 38.62 ATOM 2185 C GLU 40 33.881 47.452 11.423 10.00 38.62 ATOM 2185 C GLU 41 33.641 48.200 10.550 1.00 39.31 ATOM 2185 C GLU 41 33.641 46.875 6.000 30.30 3.00 37.26 ATOM 2195 CB LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2195 CB LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2195 CB LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2195 CB LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2195 CB LEU 41 36.507 45.380 9.954 1.00 37.57 ATOM 2195 CB CB LEU 41 36.507 45.380 9.954 1.00 37.57 ATOM 2195 CB CB LEU 41 36.507 45.380 9.954 1.00 39.38 ATOM 2195 CB CB LEU 41 36.507 45.380 9.954 1.00 39.30 3.	MOTA	2166	N	TYR	39	35.349	44.637	15.228	1.00 29	9.50	CPS3
ATOM 2169 CG TYR 39 33.219 43.106 16.996 1.00 31.89 ATOM 2170 CD1 TYR 39 32.897 40.744 16.491 1.00 34.16 ATOM 2171 CE1 TYR 39 32.897 40.744 16.491 1.00 34.63 ATOM 2173 CE2 TYR 39 33.558 42.808 18.185 1.00 32.76 ATOM 2173 CE2 TYR 39 33.558 42.808 18.185 1.00 32.76 ATOM 2173 CE2 TYR 39 33.558 42.808 18.185 1.00 32.76 ATOM 2175 CP TYR 39 33.339 40.455 17.760 1.00 33.06 ATOM 2175 CP TYR 39 33.339 40.455 17.760 1.00 33.06 ATOM 2175 CP TYR 39 33.304 43.512 18.512 1.00 36.81 ATOM 2176 C TYR 39 33.277 45.627 14.110 1.00 33.88 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.553 49.545 14.556 1.00 41.70 ATOM 2181 CG GLU 40 33.553 49.545 14.556 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.556 1.00 44.23 ATOM 2183 OEI GLU 40 33.388 47.452 11.423 1.00 38.62 ATOM 2185 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2185 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2186 CR GLU 41 33.651 46.388 11.189 1.00 38.25 ATOM 2186 CR GLU 41 33.651 46.388 11.189 1.00 37.52 ATOM 2189 CR LEU 41 33.510 46.228 9.851 1.00 37.52 ATOM 2189 CR LEU 41 37.564 46.281 9.9551 1.00 37.52 ATOM 2189 CR LEU 41 37.564 46.281 11.189 1.00 38.62 ATOM 2199 CR LEU 41 37.564 46.281 10.00 37.55 ATOM 2199 CR LEU 41 37.564 46.281 10.00 37.55 ATOM 2199 CR LEU 41 33.441 44.317 9.662 1.00 36.60 ATOM 2199 CR LEU 41 33.431 44.237 9.662 1.00 36.60 ATOM 2199 CR LEU 41 33.431 49.820 9.9551 1.00 37.57 ATOM 2199 CR LEU 41 33.431 49.820 9.9551 1.00 37.57 ATOM 2199 CR LEU 41 33.431 49.820 9.909 1.00 37.57 ATOM 2199 CR LEU 41 33.531 44.820 9.909 1.00 37.57 ATOM 2199 CR LEU 41 33.534 50.00 9.079 1.00 37.57 ATOM 2199 CR LEU 41 33.431 44.241 40.431 10.944 10.00 38.83 ATOM 2195 CR ER 42 33.537 44.251 10.903 1.00 39.30 ATOM 2195 CR ER 42 33.535 48.895 49.891 1.00 40.14 29.89 ATOM 2195 CR ER 42 33.535 47.541 10.994 10.00 38.62 ATOM 2195 CR ER 42 33.535 47.541 10.994 10.00 38.62 ATOM 2195 CR ER 42 33.53	ATOM	2167	CA	TYR	39	33.910	44.575	15.018	1.00 31	1.58	CPS3
ATOM 2171 CD1 TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2171 CD1 TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2172 CD2 TYR 39 33.658 42.808 18.185 1.00 32.76 ATOM 2173 CE2 TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.723 41.472 18.627 1.00 32.49 ATOM 2175 OH TYR 39 33.727 45.627 14.110 1.00 33.06 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2178 N GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.656 1.00 34.70 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 44.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 44.70 ATOM 2183 OEI GLU 40 33.534 49.545 14.656 1.00 44.70 ATOM 2184 OEZ GLU 40 33.538 47.452 11.423 1.00 39.62 ATOM 2186 C G GLU 40 33.888 47.452 11.423 1.00 39.62 ATOM 2186 C G GLU 40 33.898 47.452 11.423 1.00 39.63 ATOM 2188 C A LEU 41 34.651 46.388 11.189 1.00 38.62 ATOM 2188 C A LEU 41 36.507 45.380 9.954 11.00 37.52 ATOM 2189 C G LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2199 C G LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2191 CD1 LEU 41 37.754 46.251 10.003 1.00 37.52 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 37.754 46.251 10.003 1.00 37.56 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2190 C G LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2191 C D LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2192 C D LEU 41 36.507 45.380 9.954 1.00 36.05 ATOM 2190	ATOM	2168	CB	TYR	39	33.195	44.515	16.367	1.00 31	1.24	CPS3
ATOM 2170 CD1 TYR 39 32.839 42.054 16.068 1.00 34.16 ATOM 2171 CE1 TYR 39 32.839 40.744 16.491 1.00 34.63 ATOM 2172 CD2 TYR 39 33.658 42.808 18.855 1.00 32.76 ATOM 2173 CE2 TYR 39 33.658 42.808 18.855 1.00 32.76 ATOM 2174 CZ TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.404 39.126 18.112 1.00 33.06 ATOM 2175 OH TYR 39 33.404 39.126 18.112 1.00 33.06 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 34.54 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2178 N GLU 40 33.059 47.709 12.882 1.00 37.60 ATOM 2190 CB GLU 40 33.059 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.538 47.452 11.423 1.00 38.62 ATOM 2186 CB GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2186 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2186 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2186 C GLU 40 33.491 48.200 10.550 1.00 39.31 ATOM 2188 CA LEU 41 33.651 46.388 11.89 1.00 38.25 ATOM 2189 CG LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2189 CG LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2191 CD1 LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2192 CD2 LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.00 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.88 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.88 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.88 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.705 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.705 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.705 ATOM 2190 CG LEU 41 37.520 47.514 10.794 1.00 39.705 ATOM 2190 CG LEU	ATOM	2169	CG	TYR	39	33.219	43.106	16.896			CPS3
ATOM 2172 CD2 TYR 39 33.2897 40.744 16.491 1.00 34.63 ATOM 2172 CD2 TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.349 40.455 17.760 1.00 33.06 ATOM 2175 OH TYR 39 33.349 40.455 17.760 1.00 33.06 ATOM 2175 OH TYR 39 33.277 45.627 14.110 1.00 33.88 ATOM 2177 O TYR 39 33.277 45.627 14.110 1.00 33.88 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 CB GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 CB GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 CB GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 OE2 GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 OE2 GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 OE2 GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 OE2 GLU 40 33.535 49.545 14.656 1.00 44.23 ATOM 2180 OE2 GLU 40 33.535 49.545 14.656 1.00 44.23 ATOM 2180 OE2 GLU 40 33.515 48.895 15.706 1.00 44.23 ATOM 2180 OE2 GLU 40 33.515 48.895 15.706 1.00 44.59 ATOM 2180 OE2 GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2180 OE2 GLU 40 33.491 48.200 10.530 1.00 39.33 ATOM 2180 CB LEU 41 35.520 46.028 9.851 1.00 33.31 ATOM 2189 CB LEU 41 35.520 46.028 9.851 1.00 33.52 ATOM 2189 CB LEU 41 35.507 45.380 9.954 1.00 36.60 ATOM 2190 CB LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2191 CD1 LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2193 C LEU 41 33.491 48.200 10.530 1.00 37.52 ATOM 2193 C LEU 41 33.494 44.517 9.662 1.00 36.60 ATOM 2193 C LEU 41 33.494 44.517 9.662 1.00 36.60 ATOM 2193 C LEU 41 33.494 44.517 9.662 1.00 36.05 ATOM 2194 O LEU 41 33.494 44.517 9.662 1.00 36.60 ATOM 2195 N SER 42 33.537 44.251 10.00 31.00 37.52 ATOM 2194 O LEU 41 33.494 44.517 9.662 1.00 39.21 ATOM 2195 N SER 42 33.537 44.251 10.00 31.90 37.57 ATOM 2194 O LEU 41 33.494 40.495 9.555 1.00 42.27 ATOM 2194 O LEU 41 33.495 40.604 9.955 9.00 9.00 9.00 9.00 9.00 ATOM 2200 C SER 42 33.537 44.251 0.00 9.00 9.00 9.00 9.00 ATOM 2200 C CA ALA 43 33.895 40.881 4.985 5.00 9.00 9.00 9	ATOM	2170	CD1	TYR	39	32.839	42.054	16.068	1.00 34	4.16	CPS3
ATOM 2173 CE2 TYR 39 33.658 42.808 18.855 1.00 32.76 ATOM 2173 CE2 TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2174 CZ TYR 39 33.339 40.455 17.760 1.00 33.06 ATOM 2175 OH TYR 39 33.3404 39.126 18.112 1.00 36.81 ATOM 2176 C TYR 39 33.277 45.627 14.110 1.00 33.08 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2178 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.838 47.452 11.423 1.00 38.62 ATOM 2183 OEI GLU 40 33.898 47.452 11.423 1.00 38.62 ATOM 2186 CB GLU 40 33.898 47.452 11.423 1.00 38.62 ATOM 2186 CB GLU 40 33.898 47.452 11.423 1.00 38.62 ATOM 2186 CB GLU 40 33.898 47.452 11.423 1.00 38.62 ATOM 2188 CA LEU 41 33.636 46.386 11.899 1.00 46.21 ATOM 2189 CB LEU 41 35.120 46.028 9.851 1.00 37.52 ATOM 2189 CB LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2191 CD LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2192 CD LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2193 C LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2199 CB LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2199 C CB LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2199 C CB LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2199 C CB LEU 41 37.764 46.251 10.003 1.00 37.56 ATOM 2191 CD LEU 41 37.764 46.251 10.003 1.00 37.56 ATOM 2192 CD LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2193 C LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2191 CD LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2192 CD LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2193 C LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2191 CD LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM 2190 C CB LEU 41 37.764 46.251 10.003 1.00 37.57 ATOM	ATOM	2171	CE1	TYR	39	32.897	40.744	16.491			CPS3
ATOM 2174 CZ TYR 39 33.722 41.472 18.627 1.00 32.49 ATOM 2176 CZ TYR 39 33.072 41.472 18.627 1.00 32.49 ATOM 2175 OH TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2176 C TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2177 O TYR 39 32.212 45.884 13.715 1.00 36.81 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.84 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2181 CG GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2183 OEI GLU 40 33.535 49.545 14.656 1.00 41.70 ATOM 2180 OEZ GLU 40 33.515 48.895 15.706 1.00 44.23 ATOM 2180 OEZ GLU 40 33.515 48.895 15.706 1.00 44.23 ATOM 2180 OEZ GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2185 C GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2186 O GLU 41 33.491 48.200 10.530 1.00 39.31 ATOM 2188 CA LEU 41 35.120 46.028 9.851 1.00 33.55 ATOM 2189 CB LEU 41 36.507 45.380 9.954 1.00 36.60 ATOM 2199 CB LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2191 CD1 LEU 41 37.754 46.251 10.003 1.00 37.26 ATOM 2193 C LEU 41 33.206 45.380 10.604 1.00 35.48 ATOM 2193 C LEU 41 33.206 45.800 9.079 1.00 37.57 ATOM 2194 O LEU 41 33.406 45.800 9.079 1.00 37.57 ATOM 2195 N SER 42 33.574 4.251 10.003 1.00 37.57 ATOM 2196 CB SER 42 33.573 44.585 10.604 1.00 35.48 ATOM 2199 C SER 42 33.573 44.585 10.604 1.00 35.48 ATOM 2199 C SER 42 33.573 44.585 10.604 1.00 35.48 ATOM 2199 C SER 42 33.573 44.585 10.604 1.00 35.48 ATOM 2199 C SER 42 33.573 44.585 5.055 1.00 42.27 ATOM 2200 O SER 42 33.573 44.251 6.890 1.00 39.21 ATOM 2200 C SER 42 33.573 44.585 5.055 1.00 42.27 ATOM 2200 C SER 42 33.573 44.251 6.890 1.00 39.21 ATOM 2200 C SER 42 33.577 44.585 5.055 1.00 42.27 ATOM 2200 C SER 42 33.577 44.586 5.050 1.00 39.21 ATOM 2200 C SER 42 33.577 44.585 5.055 1.00 42.27 ATOM 2200 C SER 42 33.577 44.585 5.055 1.00 40.14 ATOM 2200 C SER 42 33.577 44.585 5.055 1.00 40.14 ATOM 2200 C SER 42 33.577 44.585 5.055 1.00 40.14 ATOM 2201 N ALA 43 33.886 41.485 5.055 1.00 39.21 ATOM 2202 C ALA 43 33.886 41.485 5.005 1.00 39.21 AT	ATOM	2172	CD2	TYR	39	33.658	42.808	18.185			CPS3
ATOM 2175 OF TYR 39 33.339 40.455 17.760 1.00 31.06 ATOM 2175 OF TYR 39 33.277 45.627 14.110 1.00 36.81 ATOM 2176 C TYR 39 32.122 45.484 13.715 1.00 34.54 ATOM 2178 N GLU 40 34.026 45.666 13.766 1.00 35.41 ATOM 2178 N GLU 40 33.059 47.709 12.882 1.00 37.60 ATOM 2178 OF GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.888 47.452 11.23 1.00 39.04 ATOM 2183 OEI GLU 40 33.888 47.452 11.23 1.00 39.04 ATOM 2184 OEZ GLU 40 33.888 47.452 11.23 1.00 39.62 ATOM 2185 C GLU 40 33.888 47.452 11.23 1.00 39.62 ATOM 2186 O GLU 40 33.898 47.452 11.23 1.00 39.31 ATOM 2185 C GLU 40 33.898 47.452 11.23 1.00 39.31 ATOM 2189 CB LEU 41 33.651 46.388 11.189 1.00 38.62 ATOM 2189 CB LEU 41 35.520 46.028 9.851 1.00 37.52 ATOM 2189 CB LEU 41 35.520 46.028 9.851 1.00 37.52 ATOM 2199 CG LEU 41 37.564 46.251 10.003 1.00 37.26 ATOM 2190 CG LEU 41 37.564 46.251 10.003 1.00 37.26 ATOM 2191 CD LEU 41 37.564 46.251 10.003 1.00 37.52 ATOM 2192 CD LEU 41 37.564 46.251 10.003 1.00 37.57 ATOM 2192 CD LEU 41 33.491 44.317 9.662 1.00 35.48 ATOM 2193 C LEU 41 33.491 44.317 9.662 1.00 36.60 ATOM 2193 C CD LEU 41 33.491 44.317 9.662 1.00 36.05 ATOM 2193 C CD LEU 41 33.491 44.317 9.662 1.00 36.05 ATOM 2193 C CD LEU 41 33.491 44.317 9.662 1.00 39.39 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 39.90 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 39.90 ATOM 2199 C SER 42 33.537 44.251 6.890 9.099 1.00 37.57 ATOM 2199 C SER 42 33.537 44.251 6.890 9.099 1.00 39.39 ATOM 2199 C SER 42 33.537 44.251 6.890 9.099 1.00 39.39 ATOM 2200 C SER 42 33.537 44.251 6.890 9.099 1.00 39.39 ATOM 2200 C SER 42 33.537 44.251 6.890 9.099 1.00 39.39 ATOM 2200 C SER 42 33.538 44.266 5.60 5.60 1.00 39.39 ATOM 2200 C SER 42 33.538 44.266 5.60 5.60 1.00 39.39 ATOM 2200 C C LYS 44 33.895 40.881 4.892 6.596 1.00 39.39 ATOM 2200 C C LYS 44 33.895 40.881 5.00 6.00 1.00 47.7	ATOM	2173	CE2	TYR	39	33.722	41.472				CPS3
ATOM 2175 OH TYR 39 33.404 39.126 18.112 1.00 36.81 ATOM 2176 C TYR 39 32.122 45.484 13.715 1.00 34.84 ATOM 2177 O TYR 39 32.122 45.484 13.715 1.00 34.84 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.559 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.551 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.551 49.545 14.656 1.00 41.70 ATOM 2180 CE GLU 40 33.551 49.545 14.656 1.00 44.23 ATOM 2180 CE GLU 40 33.551 49.545 14.656 1.00 44.23 ATOM 2185 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2185 C GLU 40 33.888 47.452 11.423 1.00 38.62 ATOM 2185 C GLU 40 33.881 47.452 11.423 1.00 38.62 ATOM 2187 N LEU 41 34.651 46.388 11.189 1.00 38.25 ATOM 2189 CB LEU 41 34.651 46.388 11.189 1.00 38.25 ATOM 2189 CB LEU 41 37.764 46.251 10.003 1.00 37.52 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2191 CD1 LEU 41 37.520 47.514 10.794 1.00 38.83 ATOM 2192 CD2 LEU 41 38.906 45.436 10.604 1.00 35.48 ATOM 2193 C LEU 41 38.906 45.436 10.604 1.00 35.48 ATOM 2193 C LEU 41 33.441 44.317 9.662 1.00 36.60 ATOM 2195 N SER 42 33.537 44.251 6.890 1.00 37.57 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 37.57 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.21 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.21 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.23 AT											CPS3
ATOM 2177 C TYR 39 33.277 45.627 14.110 1.00 33.88 ATOM 2178 N GLU 40 34.026 46.666 13.766 1.00 35.41 ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.553 49.545 14.656 1.00 44.23 ATOM 2183 OEI GLU 40 33.388 47.452 11.423 1.00 39.64 ATOM 2184 OEZ GLU 40 33.388 47.452 11.423 1.00 39.62 ATOM 2185 C GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2185 C GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2186 CA LEU 41 34.651 46.388 11.189 1.00 38.62 ATOM 2188 CA LEU 41 35.120 46.028 9.851 1.00 37.52 ATOM 2190 CG LEU 41 37.564 46.281 9.9551 1.00 37.52 ATOM 2190 CG LEU 41 37.564 46.281 10.00 37.26 ATOM 2191 CDL LEU 41 37.564 46.251 10.003 1.00 37.26 ATOM 2192 CD2 LEU 41 37.564 46.251 10.003 1.00 37.52 ATOM 2193 C LEU 41 33.540 47.541 10.794 10.00 38.83 ATOM 2195 N SER 42 33.537 44.251 6.890 9.079 1.00 37.57 ATOM 2193 C LEU 41 33.540 45.545 10.094 1.00 36.60 ATOM 2193 C CLEU 41 33.540 45.545 10.00 30.00 39.31 ATOM 2195 N SER 42 33.537 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C SER 42 33.537 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C SER 42 33.537 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C SER 42 33.537 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C C LEU 41 33.491 44.517 9.662 1.00 36.05 ATOM 2195 C C C LEU 41 33.491 44.517 9.662 1.00 36.05 ATOM 2195 C C C LEU 41 33.547 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C C LEU 41 33.547 44.251 6.890 9.079 1.00 37.57 ATOM 2195 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 38.96 ATOM 2195 C C C LEU 41 33.547 44.251 6.890 9.079 1.00 37.57 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 38.96 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 38.96 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 38.96 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 39.70 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 39.70 ATOM 2200 C C C LEU 41 33.548 40.453 10.00 40.14 40.00 ATOM 2200 C C LEU	ATOM		OH		39						CPS3
ATOM 2178 N GLU 40 34.026 46.666 13.766 13.00 35.41 ATOM 2178 N GLU 40 34.026 46.666 13.766 13.00 35.41 ATOM 2180 CB GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2183 OEI GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2184 OEZ GLU 40 33.551 54.855 11.00 44.23 ATOM 2185 C GLU 40 33.551 54.895 15.706 1.00 44.59 ATOM 2185 C GLU 40 33.891 48.200 10.550 1.00 39.31 ATOM 2186 C GLU 40 33.891 48.200 10.550 1.00 39.31 ATOM 2186 C GLU 40 33.491 48.200 10.550 1.00 39.31 ATOM 2187 N LEU 41 34.651 46.388 11.899 1.00 36.60 ATOM 2189 CB LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2189 CB LEU 41 36.507 45.380 9.954 1.00 37.52 ATOM 2199 CB LEU 41 37.764 46.281 10.003 1.00 37.52 ATOM 2199 CB LEU 41 37.754 46.281 10.003 1.00 37.52 ATOM 2193 C LEU 41 33.206 45.836 10.604 1.00 35.48 ATOM 2193 C LEU 41 33.206 45.836 10.604 1.00 35.48 ATOM 2193 C LEU 41 33.206 45.836 10.604 1.00 35.48 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 37.57 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 37.57 ATOM 2196 CR SER 42 33.537 44.251 6.890 1.00 37.57 ATOM 2196 CR SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2199 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER 42 33.537 44.251 6.890 1.00 38.95 ATOM 2200 C SER											CPS3
ATOM 2179 CA GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2180 CB GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.509 47.709 12.882 1.00 37.60 ATOM 2181 CG GLU 40 33.553 49.545 14.656 1.00 41.70 ATOM 2182 CD GLU 40 32.040 49.515 14.755 1.00 44.23 ATOM 2183 OEL GLU 40 33.533 49.545 15.706 1.00 44.23 ATOM 2184 OEL GLU 40 33.353 48.895 15.706 1.00 44.59 ATOM 2185 C GLU 40 33.388 47.452 11.423 1.00 38.62 ATOM 2185 C GLU 40 33.898 47.452 11.423 1.00 38.62 ATOM 2186 O GLU 40 33.491 48.200 10.530 1.00 39.31 ATOM 2187 N LEU 41 34.651 46.388 11.189 1.00 38.25 ATOM 2188 CA LEU 41 35.120 46.028 9.851 1.00 37.52 ATOM 2189 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2190 CG LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2190 CG LEU 41 37.520 47.514 10.794 10.00 38.83 ATOM 2192 CD2 LEU 41 38.906 45.436 10.604 1.00 35.48 ATOM 2193 C LEU 41 33.441 44.317 9.662 1.00 36.05 ATOM 2194 O LEU 41 33.441 44.317 9.662 1.00 36.05 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 36.05 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 38.96 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 38.96 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.70 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.70 ATOM 2195 C SER 42 33.537 44.251 6.890 1.00 39.70 ATOM 2190 C SER 42 33.538 44.668 5.434 1.00 40.14 ATOM 2195 C SER 42 33.538 44.668 5.434 1.00 40.14 ATOM 2195 C SER 42 33.538 44.668 5.434 1.00 40.14 ATOM 2195 C SER 42 33.538 44.668 5.435 1.00 39.70 ATOM 2200 C SER 42 33.138 42.665 7.641 1.00 39.70 ATOM 2200 C SER 42 33.838 44.646 5.721 1.00 30.90 39.70 ATOM 2200 C SER 42 33.838 44.646 5.721 1.00 30.90 39.70 ATOM 2200 C SER 42 33.838 44.646 5.721 1.00 40.14 ATOM 2201 N ALA 43 33.884 40.463 6.721 1.00 40.14 ATOM 2202 C ALA 43 33.884 40.463 6.721 1.00 40.14 ATOM 2203 C B ALA 43 33.884 40.463 6.721 1.00 40.40 ATOM 2200 C C ALA 43 33.884 40.463 6.721 1.00 40.40 ATOM 2202 C C ALA 43 33.885 41.842 6.596 1.00 39.90 ATOM 2202 C C ALA 43 33.885 41.842 6.596 1.00 39.90 ATOM 2202 C C ALA 43 33.895 41.845 5.096 1.											CPS3
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ATOM 2191 CD1 LEU 41 37.764 46.251 10.003 1.00 37.26 ATOM 2191 CD1 LEU 41 38.906 45.436 10.604 1.00 38.83 ATOM 2192 CD2 LEU 41 38.906 45.436 10.604 1.00 35.48 ATOM 2193 C LEU 41 38.906 45.436 10.604 1.00 35.48 ATOM 2194 O LEU 41 33.431 44.317 9.662 1.00 36.05 ATOM 2195 N SER 42 34.312 45.127 7.755 1.00 38.63 ATOM 2196 CA SER 42 33.537 44.251 6.890 1.00 38.96 ATOM 2197 CB SER 42 33.712 44.668 5.434 1.00 40.14 ATOM 2198 OG SER 42 33.712 44.668 5.434 1.00 40.14 ATOM 2199 C SER 42 33.712 44.668 5.434 1.00 40.14 ATOM 2199 C SER 42 33.3712 44.668 5.434 1.00 40.14 ATOM 2199 C SER 42 33.3712 44.668 5.434 1.00 40.14 ATOM 2199 C SER 42 33.33.84 40.64 5.906 1.00 39.70 ATOM 2200 O SER 42 35.038 44.585 5.055 1.00 39.70 ATOM 2201 N ALA 43 33.385 41.842 6.596 1.00 39.71 ATOM 2202 CA ALA 43 33.844 40.463 6.721 1.00 40.19 ATOM 2203 CB ALA 43 33.844 40.463 6.721 1.00 40.19 ATOM 2204 C ALA 43 33.844 40.463 6.721 1.00 40.48 ATOM 2205 O ALA 43 33.844 93.527 6.040 1.00 41.29 ATOM 2206 N LYS 44 36.786 40.767 4.305 1.00 40.37 ATOM 2207 CA LYS 44 36.786 40.767 4.305 1.00 40.37 ATOM 2209 CG LYS 44 38.039 41.314 2.139 1.00 40.357 ATOM 2209 CG LYS 44 38.039 41.314 2.139 1.00 40.357 ATOM 2201 CD LYS 44 39.309 41.314 2.139 1.00 45.09 ATOM 2210 CD LYS 44 39.309 41.314 2.139 1.00 45.09 ATOM 2211 CE LYS 44 39.309 41.314 2.139 1.00 45.09 ATOM 2212 NZ LYS 44 39.309 41.145 5.096 1.00 39.09 ATOM 2212 NZ LYS 44 39.309 41.145 5.096 1.00 39.09 ATOM 2212 NZ LYS 44 39.309 41.154 5.096 1.00 39.09 ATOM 2212 NZ LYS 44 39.309 41.154 5.096 1.00 37.74 ATOM 2212 NZ LYS 44 39.309 41.154 5.096 1.00 37.74 ATOM 2212 NZ LYS 44 38.095 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.095 40.886 6.226 1.00 37.74 ATOM 2212 NZ LYS 44 38.095 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.935 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.935 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.935 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.935 40.881 5.308 1.00 37.74 ATOM 2212 NZ LYS 44 38.935 40.881 5.308 1.00 37.74 ATOM 2218 CG ARG 45 38.693 45.480 6.221 1.00 45.35											CPS3
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ATOM 2209 CG LYS 44 38.039 41.314 2.339 1.00 45.09 ATOM 2210 CD LYS 44 39.309 42.177 0.145 1.00 49.05 ATOM 2211 CE LYS 44 39.309 42.177 0.145 1.00 49.05 ATOM 2212 NZ LYS 44 39.300 43.158 -0.980 1.00 50.90 ATOM 2213 C LYS 44 39.300 43.158 -0.980 1.00 50.90 ATOM 2213 C LYS 44 39.306 43.158 5.308 1.00 39.09 ATOM 2214 O LYS 44 38.955 40.881 5.308 1.00 39.09 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 37.74 ATOM 2217 CB ARG 45 38.594 43.460 6.291 1.00 37.61 ATOM 2218 CG ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.095 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2210 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41											CPS3
ATOM 2210 CD LYS 44 37.958 42.106 0.840 1.00 47.76 ATOM 2211 CE LYS 44 39.309 42.177 0.145 1.00 49.05 ATOM 2212 NZ LYS 44 39.300 43.158 -0.980 1.00 50.90 ATOM 2213 C LYS 44 39.309 43.158 -0.980 1.00 50.90 ATOM 2214 O LYS 44 38.955 40.881 5.308 1.00 39.00 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.233 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 41.25 ATOM 2219 CD ARG 45 40.264 6.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 45.41											CPS3
ATOM 2211 CE LYS 44 39.309 42.177 0.145 1.00 49.05 ATOM 2212 NZ LYS 44 39.309 42.177 0.145 1.00 49.05 ATOM 2213 C LYS 44 37.886 41.454 5.097 1.00 39.09 ATOM 2214 O LYS 44 38.955 40.881 5.308 1.00 39.09 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 39.00 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 37.74 ATOM 2217 CB ARG 45 38.594 43.460 6.291 1.00 37.61 ATOM 2218 CG ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.93 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 45.41											CPS3
ATOM 2213 CZ LYS 44 39.300 43.158 -0.980 1.00 50.90 ATOM 2213 CZ LYS 44 38.955 40.881 5.308 1.00 39.00 ATOM 2214 CD LYS 44 38.955 40.881 5.308 1.00 39.00 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.073 44.882 6.517 1.00 41.25 ATOM 2218 CG ARG 45 38.093 46.334 5.076 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.334 5.076 1.00 45.35 ATOM 2210 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.351								0.840			CPS3
ATOM 2213 C LYS 44 37.886 41.454 5.097 1.00 39.09 ATOM 2214 O LYS 44 38.955 40.881 5.308 1.00 39.00 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41							42.177	0.145	1.00 49	9.05	CPS3
ATOM 2214 O LYS 44 38.955 40.881 5.308 1.00 39.00 ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.23 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41							43.158	-0.980	1.00 50	0.90	CPS3
ATOM 2215 N ARG 45 37.625 42.687 5.518 1.00 37.74 ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.073 44.882 6.517 1.00 41.25 ATOM 2219 CD ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2220 NE ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2221 CZ ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41						37.886	41.454	5.097	1.00 39	9.09	CPS3
ATOM 2216 CA ARG 45 38.594 43.460 6.291 1.00 36.13 ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41							40.881	5.308	1.00 39	9.00	CPS3
ATOM 2217 CB ARG 45 38.073 44.882 6.517 1.00 37.61 ATOM 2218 CG ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41						37.625	42.687	5.518	1.00 37	7.74	CPS3
ATOM 2218 CG ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41						38.594	43.460	6.291	1.00 36	5.13	CPS3
ATOM 2218 CG ARG 45 38.223 45.805 5.314 1.00 41.25 ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41					45	38.073	44.882	6.517	1.00 37	7.61	CPS3
ATOM 2219 CD ARG 45 39.693 46.134 5.076 1.00 43.51 ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41					45	38.223	45.805		1.00 41	1.25	CPS3
ATOM 2220 NE ARG 45 40.264 46.872 6.203 1.00 45.35 ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41					45	39.693		5.076	1.00 43	3.51	CPS3
ATOM 2221 CZ ARG 45 41.392 46.536 6.826 1.00 46.41					45	40.264			1.00 45	5.35	CPS3
					45	41.392					CPS3
	ATOM	2222	NH1	ARG	45	42.078	45.469	6.435			CPS3



SEP 0 9 2002

FIG. 1A-39

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APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSHAM

ATOM	2223	NH2	ARG	45	41.833	47.269	7.843	1.00 46.62	CPS3
ATOM	2224	C	ARG	45	38.909	42.799	7.634	1.00 34.32	
ATOM									CPS3
	2225	0	ARG	45	40.049	42.842	8.097	1.00 32.42	CPS3
ATOM	2226	N	LYS	46	37.899	42.188	8.251	1.00 32.83	CPS3
ATOM	2227	CA	LYS	46	38.075	41.509	9.532	1.00 31.12	CPS3
ATOM	2228	CB	LYS	46	36.775	40.842	9.987	1.00 31.02	CPS3
ATOM	2229	CG	LYS	46	35.746	41.775	10.599	1.00 30.98	CPS3
ATOM	2230	CD	LYS	46	34.553	40.977	11.100	1.00 32.86	CPS3
ATOM	2231	CE	LYS	46	33.524	41.861	11.785	1.00 34.98	CPS3
ATOM	2232	NZ	LYS	46	32.360	41.053	12.230	1.00 37.21	CPS3
ATOM	2233	C	LYS	46	39.148	40.438	9.434	1.00 30.57	CPS3
ATOM	2234	ō	LYS	46	40.025	40.352	10.293	1.00 28.78	CPS3
ATOM	2235	N	ASN	47	39.061	39.612	8.392	1.00 29.54	CPS3
ATOM	2236	CA		47					
			ASN		40.020	38.533	8.186	1.00 29.84	CPS3
ATOM	2237	CB	ASN	47	39.589	37.671	6.989	1.00 31.31	CPS3
ATOM	2238	CG	ASN	47	40.603	36.588	6.635	1.00 33.49	CPS3
ATOM	2239		ASN	47	40.838	35.651	7.400	1.00 34.63	CPS3
MOTA	2240	ND2		47	41.201	36.713	5.461	1.00 34.30	CPS3
MOTA	2241	С	ASN	47	41.436	39.083	7.976	1.00 28.84	CPS3
ATOM	2242	0	ASN	47	42.401	38.521	8.501	1.00 27.85	CPS3
ATOM	2243	N	GLU	48	41.562	40.174	7.224	1.00 27.20	CPS3
ATOM	2244	CA	GLU	48	42.881	40.779	6.988	1.00 27.86	CPS3
ATOM	2245	CB	GLU	48	42.795	41.910	5.955	1.00 30.08	CPS3
ATOM	2246	CG	GLU	48	42.315	41.492	4.580	1.00 34.36	CPS3
ATOM	2247	CD	GLU	48	41.937	42.687	3.716	1.00 34.33	CPS3
ATOM	2248		GLU	48	41.356	42.477	2.627	1.00 40.99	
ATOM	2249		GLU						CPS3
ATOM				48	42.221	43.835	4.124	1.00 39.72	CPS3
	2250	С	GLU	48	43.451	41.363	8.285	1.00 25.90	CPS3
ATOM	2251	0	GLU	48	44.633	41.197	8.589	1.00 24.51	CPS3
ATOM	2252	N	PHE	49	42.601	42.065	9.030	1.00 24.05	CPS3
ATOM	2253	CA	PHE	49	42.995	42.688	10.293	1.00 24.45	CPS3
ATOM	2254	CB	PHE	49	41.809	43.473	10.866	1.00 25.52	CPS3
ATOM	2255	CG	PHE	49	42.073	44.119	12.203	1.00 26.02	CPS3
ATOM	2256	CD1	PHE	49	42.503	45.440	12.285	1.00 26.53	CPS3
ATOM	2257	CD2	PHE	49	41.842	43.419	13.385	1.00 26.09	CPS3
ATOM	2258	CE1	PHE	49	42.688	46.061	13.529	1.00 26.57	CPS3
ATOM	2259	CE2	PHE	49	42.028	44.027	14.630	1.00 25.34	CPS3
ATOM	2260	CZ	PHE	49	42.448	45.350	14.702	1.00 24.86	CPS3
ATOM	2261	c	PHE	49	43.431	41.603	11.278	1.00 24.05	
ATOM	2262	ō	PHE	49	44.499				CPS3
ATOM	2263	N				41.691	11.885	1.00 22.16	CPS3
ATOM			LEU	50	42.597	40.577	11.429	1.00 23.09	CPS3
	2264	CA	LEU	50	42.894	39.478	12.342	1.00 23.23	CPS3
ATOM	2265	CB	LEU	50	41.727	38.488	12.348	1.00 24.42	CPS3
ATOM	2266	CG	LEU	50	41.788	37.294	13.297	1.00 26.20	CPS3
MOTA	2267		LEU	50	42.039	37.735	14.751	1.00 26.62	CPS3
ATOM	2268	CD2	LEU	50	40.468	36.551	13.182	1.00 27.72	CPS3
ATOM	2269	С	LEU	50	44.191	38.758	11.970	1.00 22.25	CPS3
ATOM	2270	0	LEU	50	45.033	38.483	12.835	1.00 21.88	CPS3
ATOM	2271	N	ALA	51	44.359	38.455	10.685	1.00 21.04	CPS3
ATOM	2272	CA	ALA	51	45.564	37.773	10.223	1.00 20.88	CPS3
ATOM	2273	CB	ALA	51	45.460	37.467	8.727	1.00 20.00	CPS3
ATOM	2274	C	ALA	51					
ATOM	2275	0	ALA		46.815	38.615	10.497	1.00 21.09	CPS3
ATOM	2275	N		51	47.860	38.077	10.863	1.00 20.76	CPS3
			GLY	52	46.698	39.929	10.321	1.00 21.47	CPS3
ATOM	2277	CA	GLY	52	47.830	40.814	10.559	1.00 20.85	CPS3
ATOM	2278	С	GLY	52	48.230	40.871	12.026	1.00 21.87	CPS3
ATOM	2279	0	GLY	52	49.420	40.891	12.355	1.00 20.94	CPS3



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FIG. 1A-40

48.429

48.731

47.196

50.296

51.291

52.121

53.210

52.745

53.869

51.864

50.484

49.741

48.445

47.650

46.589

52.694

53.456

52.555

53.343

52.885

52.985

52.321

51.079

53.059

54.818

55.696

55.089

56.458

56.491

57.011

58.160

56.200

52.490 40.382

41.015

41.049

37.492

37.248

36.692

35.477

34.710

33.214

32.682

32.744

32.207

35.900

35.365

36.867

37.353

38.461

37.883

37.595

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ATOM 2280 N ARG 53 ATOM 2281 CA ARG 53 ATOM 2282 CB ARG 53 ATOM 2283 CG ARG 53 516 ATOM 2284 CD ARG 53

ATOM 2285 NE ARG 53 ATOM 2286 cz ARG 53 ATOM 2287 NH1 ARG 53 ATOM 2288 NH2 ARG 53 ATOM 2289 C ARG 53 ATOM 2290 0 ARG 53 ATOM 2291 N PHE 54 ATOM 2292 CA PHE 54 ATOM 2293 CB PHE 54 54

ATOM 2294 CG PHE ATOM 2295 CD1 PHE 54 ATOM 2296 CD2 PHE 54 ATOM 2297 CE1 PHE 54 ATOM 2298 CE2 PHE 54 ATOM 2299 CZ DHE 54 MOTA 2300 C PHE 54

> 2301 0 PHE

2302 N ALA **5**5

2303 CA A.TA

2304 CB ALA

2305 С ALA 55

2306 0 ALA 55

2307 N ALA 56

ATOM

ATOM 2308 CA AT.A ATOM 2309 CB ALA ATOM 2310 С ALA ATOM 2311 0 AT.A ATOM 2312 N LYS ATOM 2313 CA LYS ATOM 2314 CB LYS ATOM 2315 CG LYS ATOM 2316 CD LYS ATOM 2317 CE LYS ATOM 2318 NZ LYS ATOM 2319 С LYS ATOM 2320 0 LYS ATOM 2321 N GLU

2322 CA GLU

2323 CB GLU

2324 CG GLU

2325 CD GLU

2326

ATOM 2327 OE2 GLU 58 ATOM 2328 C GLU 58 MOTA 2329 0 GLU 58 ATOM 2330 N ALA 59 ATOM 2331 CA ALA 59 ATOM 2332 CB ALA 59 ATOM 2333 С ALA 59 ATOM 2334 0 ALA 59 ATOM 2335 N PHE 60 ATOM 2336 CA PHE 60

OE1 GLU

47.234 40.907 12.908 47.489 40.953 14.344 46.188 41.249 15.102 45.749 42.697 15.023 46.854 43.589 15.542 46.364 44.864 46.020 45.905

16.046 15.293 46.104 45.841 13.967 45.615 47.028 15.882 48.067 39.628 14.802 48.983 39.585 15.623 47.524 38.541 14.274 48.001 37.214 14.639

47.145 36.157 13.926 47.514 34.736 14.248 34.050 13.462 46.903 34.068 15.305 32.726 13.713 32.735 15.572 48.113 32.061 14.773 1.00 26.02 49.480 37.082 14.254

36.615 15.049 49.818 37.512 13.042 51.202 37.426 12.564 37.903 11.110 38.271 13.439 1.00 17.75 37.833 13.822 1.00 17.44 51.678 39.481 13.755 1.00 17.64

14.572

1.00 17.27

51.828 41.769 14.651 1.00 17.54 39.840 15.978 1.00 18.48 39.927 16.492 1.00 16.93 51.710 39.278 16.600 1.00 17.56 38.758 17.953 1.00 17.39 38.545 18.593 1.00 17.01 39.852 18.728 1.00 17.00 39.709

19.516 1.00 17.39 19.466 1.00 17.65 20.526 1.00 18.42 17.958 1.00 18.30 18.895 1.00 17.97 16,903 1.00 19.29 16.770 1.00 21.29

15.518 1.00 25.54 15.639 1.00 35.02 16.899 1.00 36.12 17.033 1.00 40.18 17.772 16.644 17.335

1.00 38.83 1.00 20.21 15.768 15.580 14.521 16.900

17.271 1.00 17.74 17.613 1.00 16.51 56.655 39.219 18.882 1.00 17.55

1.00 19.40 1.00 16.40 1.00 17.36 1.00 17.44 1.00 17.42

CPS3 CPS3 CPS3 CPS3 CPS3 CPS3

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1.00 20.71

1.00 19.99

1.00 21.12 CPS3 1.00 25.14 CDG3 1.00 26.59 CPS3 1.00 29.01 CPS3 1.00 29.46 CPS3 1.00 29.27 CPS3

CPS3

CDS3

1.00 26.91 CPS3 1.00 18.67 CPS3 1.00 19.03 CPS3 1.00 19.10 CPS3 1.00 18.17 CPS3

1.00 20.62 CPS3 1.00 21.61 CPS3 1.00 22.92 CPS3

1.00 23.51 CPS3 1.00 24.49 CPS3 1.00 24.31 CPS3 CPS3

1.00 18.48 CPS3 1.00 16.83 CPS3 1.00 18.82 CPS3 1.00 19.23 CPS3 1.00 19.19 CPS3

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-	<u>5</u>	SUBCLASS	
At he was an a property of	C.G. F	CLASS.	
A	PPROVED :	25	MFTSKAM

ATOM	2337	СВ	PHE	60	55.586	40.128	19.502	1.00 17.91	CPS3
ATOM	2338	CG	PHE	60	55.984	40.684	20.847	1.00 18.76	CPS3
ATOM	2339	CD1	PHE	60	56.755	41.838	20.933	1.00 18.58	CPS3
ATOM	2340	CD2	PHE	60	55.659	40.001	22.021	1.00 19.49	CPS3
ATOM	2341		PHE	60	57.212	42.309	22.172	1.00 20.20	CPS3
ATOM	2342	CE2	PHE	60	56.107	40.459	23.266	1.00 20.93	CPS3
ATOM	2343	CZ	PHE	60	56.886	41.612	23.341	1.00 20.99	CPS3
ATOM	2344	С	PHE	60	57.008	38.118	19.883	1.00 18.91	CPS3
ATOM	2345	0	PHE	60	58.053	38.173	20.543	1.00 18.95	CPS3
ATOM	2346	N	SER	61	56.137	37.123	20.001	1.00 18.23	CPS3
ATOM	2347	CA	SER	61	56.370	36.036	20.946	1.00 19.91	CPS3
ATOM	2348	CB	SER	61	55.167	35.081	20.978	1.00 20.94	CPS3
ATOM	2349	OG	SER	61	55.170	34.217	19.851	1.00 25.41	CPS3
ATOM	2350	C	SER	61	57.642	35.256	20.618	1.00 21.39	CPS3
ATOM	2351	0	SER	61	58.278	34.697	21.511	1.00 21.46	CPS3
ATOM	2352	N	LYS	62	58.011	35.206	19.345	1.00 20.86	CPS3
ATOM	2353	CA	LYS	62	59.227	34.500	18.958	1.00 23.14	CPS3
ATOM	2354	CB	LYS	62	59.239	34.237	17.455	1.00 24.31	CPS3
ATOM	2355	CG	LYS	62	58.295	33.143	17.003	1.00 28.06	CPS3
ATOM	2356	CD	LYS	62	58.340	33.057	15.490	1.00 32.02	CPS3
ATOM	2357	CE	LYS	62	58.060	31.655	14.987	1.00 34.92	CPS3
ATOM	2358	NZ	LYS	62	58.159	31.623	13.510	1.00 35.49	CPS3
ATOM	2359	С	LYS	62	60.444	35.343	19.340	1.00 22.30	CPS3
ATOM	2360	0	LYS	62	61.464	34.815	19.788	1.00 23.20	CPS3
ATOM	2361	N	ALA	63	60.337	36.654	19.156	1.00 19.62	CPS3
ATOM	2362	CA	ALA	63	61.437	37.547	19.512	1.00 20.06	CPS3
ATOM	2363	CB	ALA	63	61.145	38.960	19.019	1.00 20.10	CPS3
MOTA	2364	C	ALA	63	61.603	37.543	21.035	1.00 21.63	CPS3
ATOM	2365	0	ALA	63	62.724	37.529	21.550	1.00 23.66	CPS3
ATOM	2366	N	PHE	64	60.480	37.536	21.749	1.00 20.52	CPS3
ATOM	2367	CA	PHE	64	60.502	37.548	23.209	1.00 23.24	CPS3
ATOM	2368	CB	PHE	64	59.079	37.690	23.752	1.00 23.53	CPS3
ATOM	2369	CG	PHE	64	59.023	38.051	25.211	1.00 24.99	CPS3
ATOM	2370	CD1	PHE	64	59.492	39.283	25.653	1.00 26.02	CPS3
MOTA	2371	CD2	PHE	64	58.488	37.163	26.135	1.00 25.12	CPS3
MOTA	2372		PHE	64	59.423	39.632	27.008	1.00 28.33	CPS3
ATOM	2373		PHE	64	58.412	37.495	27.484	1.00 26.52	CPS3
ATOM	2374	CZ	PHE	64	58.87 7	38.729	27.924	1.00 27.24	CPS3
ATOM	2375	С	PHE	64	61.140	36.251	23.718	1.00 25.44	CPS3
MOTA	2376	0	PHE	64	61.688	36.204	24.826	1.00 24.64	CPS3
ATOM	2377	N	GLY	65	61.039	35.202	22.910	1.00 26.62	CPS3
MOTA	2378	CA	GLY	65	61.662	33.938	23.255	1.00 30.83	CPS3
ATOM	2379	С	GLY	65	60.802	32.879	23.912	1.00 32.24	CPS3
ATOM	2380	0	GLY	65	61.209	31.719	23.980	1.00 33.69	CPS3
ATOM	2381	N	THR	66	59.616	33.256	24.376	1.00 32.78	CPS3
ATOM	2382	CA	THR	66	58.733	32.302	25.043	1.00 34.27	CPS3
ATOM	2383	CB	THR	66	57.991	32.969	26.200	1.00 35.66	CPS3
ATOM	2384	OG1		66	57.122	33.978	25.668	1.00 37.64	CPS3
ATOM	2385		THR	66	58.969	33.610	27.179	1.00 34.33	CPS3
ATOM	2386	С	THR	66	57.663	31.691	24.143	1.00 34.55	CPS3
ATOM	2387	0	THR	66	57.154	30.610	24.431	1.00 34.19	CPS3
ATOM	2388	N	GLY	67	57.320	32.376	23.054	1.00 34.33	CPS3
ATOM	2389	CA	GLY	67	56.256	31.877	22.198	1.00 34.53	CPS3
ATOM	2390	C	GLY	67	54.962	32.175	22.945	1.00 34.85	CPS3
ATOM	2391	0	GLY	67	55.012	32.656	24.080	1.00 34.24	CPS3
ATOM	2392	N	ILE	68	53.808	31.915	22.338	1.00 35.31	CPS3
ATOM	2393	CA	ILE	68	52.537	32.175	23.016	1.00 35.28	CPS3

SEP 0 9 2002

FIG. 1A-42

47.287

40.350

26,028 1.00 22.75

68

SUBCLASS ASS DRAFISMAN

TRADE!

ATOM 2394 CB ILE ATOM 2395 CG2 ILE 68 ATOM 2396 CG1 TLE 68 ATOM 2397 CD1 ILE 68 ATOM 2398 C ILE 68 ATOM 2399 0 ILE 68 ATOM 2400 N GLY 69 ATOM 2401 CA GLY 69 ATOM 2402 С GLY 69 GLY 69 ATOM 2403 0 ATOM 2404 N ALA 70 ATOM 2405 CA ALA 70 ATOM 2406 CB ALA 70 ATOM 2407 С AT.A 70 ATOM 2408 ALA 0 70 ATOM 2409 N GLN. 71 ATOM 2410 CA GLN 71 ATOM 2411 CB GLN 71 ATOM 2412 CG GLN 71 ATOM 2413 CD GLN 71 ATOM 2414 OFI GIN 71 ATOM 2415 NE2 GLN 71 ATOM 2416 С GLN 71 ATOM 2417 0 GLN 71 ATOM 2418 N LEU 72 ATOM 2419 CA LEU 72 ATOM 2420 CB LEU 72 ATOM 2421 CG LEU 72 ATOM 2422 CD1 LEU 72 ATOM 2423 CD2 LEU 72 ATOM 2424 C LEU 72 ATOM 2425 0 LEU 72 N ATOM 2426 SER 73 ATOM 2427 CA SER 73 ATOM 2428 CB SER 73 ATOM 2429 OG SER 73 ATOM 2430 С SER 73 ATOM 2431 0 SER 73 ATOM 2432 N PHE 74 ATOM 2433 CA PHE 74 ATOM 2434 CB PHE 74 ATOM 2435 CG PHE 74 ATOM 2436 CD1 PHE 74 ATOM 2437 CD2 PHE 74 ATOM 2438 CE1 PHE 74 ATOM 2439 CE2 PHE 74 ATOM 2440 CZ PHE 74 ATOM 2441 C PHE 74 ATOM 2442 O PHE 74 ATOM 2443 N GLN 75 ATOM 2444 CA GLN 75 ATOM 2445 CB GLN 75 ATOM 2446 CG GLN 75 ATOM 2447 CD GLN 75 ATOM 2448 OE1 GLN 75 ATOM 2449 NE2 GLN 75 ATOM 2450 С GLN 75

TECH CENTER 1600/2900 51.389 32.407 22.011 1.00 34.11 CPS3 50.052 32.474 22.755 1.00 32.62 CPS3 51.640 33.690 21.219 1.00 32.54 CPS3 51.647 34.958 22.063 1.00 32.72 CPS3 52.161 30.999 23.910 1.00 36.56 CPS 52.085 29.862 23.447 1.00 36.53 CPS3 1.00 36.84 51.922 31.279 25.187 CPS3 51.565 30.221 26.115 1.00 38.40 CDS3 51.481 30.700 27.550 1.00 38.69 CPS3 50.987 31.797 27.820 1.00 38.83 CDC3 51.978 29.882 28.474 1.00 38.37 CPS3 51.949 30.215 29.895 1.00 37.89 CPS3 52.510 29.043 30.710 1.00 38.76 CPS3 52.684 31.506 30.270 1.00 37.56 CPS3 1.00 37.72 52,225 32.262 31.122 CPS3 53.817 31.769 1.00 36.91 29 634 CPS3 54.590 32.965 29.954 1.00 36.41 CPS3 56.072 32.693 29.697 1.00 38.98 CPS3 56.540 31.358 30.251 1.00 42.83 CPS3 58.024 31.132 30.053 1.00 45.56 CPS3 58.854 31.783 30.695 1.00 47.59 CPS3 58.369 30.211 29.156 1.00 47.26 CPS3 54.167 34.225 29.192 1.00 33.99 CPS3 54.514 35.332 29.585 1.00 34.52 CPS3 53.422 34.056 28.107 1.00 30.98 CPS3 52.993 35.195 27.304 1.00 27.97 CPS3 54.108 35.592 26.333 1.00 26.71 CPS3 53.888 36.797 25.415 1.00 25.21 CPS 3 54.008 38.103 26.212 1.00 25.07 CPS3 54.930 36.760 24.299 1.00 26.26 CPS3 51.727 34.852 26.532 1.00 26.94 CPS3 51.679 33.877 25.779 1.00 27.79 CPS3 50.706 35.673 26.723 1.00 24.63 CPS3 49.416 35.486 26.081 1.00 24.89 CPS3 48.318 35.677 27.135 1.00 26.50 CPS3 47.068 35.913 26.531 1.00 28.99 CPS3 49.228 36.504 24.957 1.00 23.56 CPS3 49.903 37.537 24.942 1.00 22.03 CPS3 48.324 36.211 24.017 1.00 22.96 CPS3 48.016 37.150 22.933 1.00 21.51 CPS3 46.922 36.599 22.010 1.00 23.03 CPS3 47.386 35.535 21.060 1.00 24.56 CPS3 1.00 25.15 48.330 35.820 20.079 CPS3 1.00 26.66 46.854 34.246 21.127 CPS3 48.740 34.837 19.175 1.00 25.67 CPS3 47.257 33.251 20.226 1.00 27.19 CPS3 48.200 33.547 19.251 1.00 26.99 CPS3 47.476 38.424 23.573 1.00 22.00 CPS3 47.624 39.519 23.038 1.00 20.92 CPS3 46.830 38.270 24.726 1.00 22.26 CPS3 46.246 39,402 25.431 1.00 22.41 CPS3 45.313 38.895 26.543 1.00 23.41 CPS3 44.119 38.109 26.025 1.00 25.20 CPS3 43.257 38.954 25.118 1.00 26.61 CPS3 42.891 40.080 25.476 1.00 27.48 CPS3 42,928 38,429 23.938 1.00 25.82 CPS3

CPS3



SEP 0 9 2002

CPS3

13.309 1.00 31.70

12.665 1.00 34.29

10.888 1.00 38.59

16.095 1.00 21.74

1.00 36.91

1.00 22.25

49.316 52.839 14.998 1.00 22.45

48.327 52.868 13.829 1.00 25.71

50.750 54.801 15.048 1.00 21.32 51.055 56.169 15.411 1.00 24.29 52.568 56.396 15.564 1.00 23.73

11.996

15.423

47.907 51.512

49.057 50.788

48.582 49.508

47.631 49.799

49.591 54.269

48.757 54.882

TECH CENTER 1600/2900

SEP O 3 2002

ATOM

2497 CA LYS 81

2498 CB LYS 81

2499 CG

2500 CD

2501 CE

2503 C

2504 O

2505 N

2506 CA

LYS 81

LYS

LYS 81

2502 NZ LYS 81

2507 CB ASP 82

81

LYS 81

LYS 81

ASP 82

ASP 82

	ATOM	2451	0	GLN	75	46.962	41.486	26.389	1.00 21.60
	ATOM	2452	N	ASP	76	48.532	39.890	26.146	1.00 21.97
100	ATOM	2453	CA	ASP	76	49.595	40.730	26.710	1.00 22.16
AS	ATOM	2454	CB	ASP	76	50.738	39.876	27.279	1.00 22.82
	ATOM	2455	CG	ASP	76	50.332	39.058	28.494	1.00 25.52
O.G. FIG.	ATOM	2456	OD1	ASP	76	49.557	39.565	29.332	1.00 25.20
14 100	ATOM	2457	OD2	ASP	76	50.823	37.915	28.614	1.00 24.81
1 - 1 82	ATOM	2458	C	ASP	76	50.223	41.635	25.661	1.00 21.66
1215	ATOM	2459	0	ASP	76	51.059	42.481	25.982	1.00 19.63
0.0.	ATOM	2460	N	ILE	77	49.826	41.450	24.405	1.00 21.29
10 31	ATOM	2461	CA	ILE	77	50.416	42.202	23.301	
18 - 8	ATOM	2462	CB	ILE	77	51.088	41.225		1.00 19.67
APPTOVED SY ORAFTSKAN	ATOM	2463	CG2	ILE	77	51.893	41.225	22.318	1.00 19.23
1 A	ATOM	2464		ILE	77			21.253	1.00 18.53
	ATOM	2465	CD1		77	51.987	40.247	23.084	1.00 17.28
	ATOM	2466	C	ILE		52.313	38.989	22.257	1.00 19.10
	ATOM	2467	0		77	49.379	42.988	22.520	1.00 20.27
	ATOM	2468		ILE	77	48.401	42.416	22.062	1.00 20.00
	ATOM		N	GLU	78	49.603	44.288	22.354	1.00 21.09
		2469	CA	GLU	78	48.670	45.106	21.591	1.00 20.73
	ATOM	2470	CB	GLU	78	47.909	46.082	22.496	1.00 22.17
	MOTA	2471	CG	GLU	78	46.819	46.843	21.737	1.00 24.01
	ATOM	2472	CD	GLU	78	45.862	47.584	22.651	1.00 27.03
	ATOM	2473		GLU	78	46.036	48.806	22.844	1.00 28.55
	ATOM	2474		GLU	78	44.937	46.934	23.181	1.00 28.54
	ATOM	2475	С	GLU	78	49.384	45.892	20.508	1.00 20.37
	ATOM	2476	0	GLU	78	50.431	46.485	20.749	1.00 20.67
	ATOM	2477	N	ILE	79	48.826	45.877	19.303	1.00 19.96
	ATOM	2478	CA	ILE	79	49.420	46.642	18.212	1.00 19.14
	ATOM	2479	CB	ILE	79	49.368	45.860	16.850	1.00 19.23
	ATOM	2480	CG2		79	49.577	46.830	15.678	1.00 19.82
	ATOM	2481	CG1	ILE	79	50.477	44.798	16.795	1.00 21.31
	ATOM	2482	CD1	ILE	79	50.318	43.645	17.758	1.00 22.36
	ATOM	2483	C	ILE	79	48.629	47.942	18.090	1.00 20.00
	ATOM	2484	0	ILE	79	47.389	47.928	18.088	1.00 20.09
	ATOM	2485	N	ARG	80	49.340	49.068	18.028	1.00 19.20
	ATOM	2486	CA	ARG	80	48.703	50.380	17.861	1.00 20.32
	ATOM	2487	CB	ARG	80	48.924	51.258	19.107	1.00 20.53
	ATOM	2488	CG	ARG	80	48.340	50.644	20.380	
	ATOM	2489	CD	ARG	80	48.505	51.527	21.617	1.00 21.77
	ATOM	2490	NE	ARG	80	47.957	50.833		1.00 23.01
	ATOM	2491	CZ	ARG	80	48.032		22.780	1.00 23.15
	ATOM	2492	NH1		80		51.267	24.038	1.00 25.30
	ATOM	2493		ARG	80	48.634	52.412	24.321	1.00 20.84
	ATOM	2494		ARG	80	47.511	50.536	25.014	1.00 26.37
	ATOM	2495	0	ARG		49.349	51.037	16.640	1.00 20.88
	ATOM	2496	N	LYS	80	50.362	50.550	16.138	1.00 20.01
	3.000	2470	74	ni2	81	48.755	52.123	16.148	1.00 21.43



SEP 0 9 2002

FIG. 1A-44

(3	SUBCLASS	
0.6. FIG	CLASS 51	
APPROVEG	25	DRAFISMAH

ATOM	2508	CG	ASP	82	53.340	56.303	14.253	1.00 25.37	CPS3
ATOM	2509		ASP	82	52.736	56.371	13.161	1.00 25.70	CPS3
ATOM	2510		ASP	82	54.585	56.182	14.331	1.00 27.40	CPS3
ATOM	2511	С	ASP	82	50.446	57.129	14.394	1.00 26.03	CPS3
ATOM	2512	0	ASP	82	49.682	56.711	13.518	1.00 25.08	CPS3
ATOM	2513	N	GLN	83	50.783	58.406	14.521	1.00 27.30	CPS3
ATOM	2514	CA	GLN	83	50.243	59.439	13.648	1.00 30.37	CPS3
ATOM	2515	CB	GLN	83	50.694	60.810	14.158	1.00 32.92	CPS3
ATOM	2516	CG	GLN	83	50.035	61.193	15.481	1.00 36.66	CPS3
ATOM	2517	CD	GLN	83	48.633	61.738	15.292	1.00 40.09	CPS3
MOTA	2518		GLN	83	48.448	62.940	15.079	1.00 42.06	CPS3
ATOM	2519	NE2	GLN	83	47.637	60.859	15.354	1.00 40.07	CPS3
ATOM	2520	С	GLN	83	50.587	59.276	12.167	1.00 30.09	CPS3
ATOM	2521	0	GLN	83	49.900	59.834	11.308	1.00 30.34	CPS3
ATOM	2522	N	ASN	84	51.647	58.532	11.865	1.00 29.03	CPS3
ATOM	2523	CA	ASN	84	52.024	58.296	10.471	1.00 29.59	CPS3
ATOM	2524	CB	ASN	84	53.544	58.202	10.303	1.00 31.65	CPS3
ATOM	2525	CG	ASN	84	54.239	59.536	10.457	1.00 34.87	CPS3
ATOM	2526		ASN	84	53.732	60.566	10.022	1.00 36.47	CPS3
ATOM	2527		ASN	84	55.425	59.520	11.060	1.00 36.00	CPS3
ATOM	2528	C	ASN	84	51.419	56.990	9.974	1.00 28.93	CPS3
ATOM	2529	0	ASN	84	51.609	56.613	8.815	1.00 30.32	CPS3
MOTA	2530	N	GLY	85	50.712	56.286	10.852	1.00 26.33	CPS3
ATOM	2531	CA	GLY	85	50.116	55.019	10.464	1.00 24.71	CPS3
ATOM	2532	C	GLY	85	51.063	53.851	10.697	1.00 23.82	CPS3
MOTA	253 3	0	GLY	85	50.759	52.713	10.341	1.00 24.11	CPS3
ATOM	2534	N	LYS	86	52.214	54.131	11.302	1.00 21.10	CPS3
ATOM	2535	CA	LYS	86	53.204	53.096	11.582	1.00 21.62	CPS3
ATOM	2536	CB	LYS	86	54.561	53.738	11.883	1.00 21.42	CPS3
ATOM	2537	CG	LYS	86	55.625	52.760	12.401	1.00 23.00	CPS3
MOTA	2538	CD	LYS	86	56.097	51.789	11.325	1.00 22.60	CPS3
MOTA	2539	CE	LYS	86	57.073	50.766	11.921	1.00 21.76	CPS3
ATOM	2540	NZ	LYS	86	57.761	49.970	10.852	1.00 21.43	CPS3
ATOM	2541	С	LYS	86	52.782	52.244	12.783	1.00 20.36	CPS3
ATOM	2542	0	LYS	86	52.468	52.776	13.843	1.00 20.19	CPS3
ATOM	2543	N	PRO	87	52.770	50.912	12.632	1.00 20.59	CPS3
ATOM	2544	CD	PRO	87	52.925	50.084	11.423	1.00 21.13	CPS3
ATOM	2545	CA	PRO	87	52.375	50.091	13.781	1.00 20.38	CPS3
ATOM	2546	CB	PRO	87	52.082	48.729	13.160	1.00 22.01	CPS3
ATOM	2547	CG	PRO	87	53.044	48.675	12.009	1.00 23.44	CPS3
ATOM	2548	С	PRO	87	53.481	49.991	14.812	1.00 18.94	CPS3
ATOM	2549	0	PRO	87	54.662	49.996	14.468	1.00 18.59	CPS3
ATOM ATOM	2550	N	TYR	88	53.092	49.938	16.082	1.00 18.68	CPS3
ATOM	2551	CA	TYR	88	54.064	49.757	17.155	1.00 18.87	CPS3
ATOM	2552	CB	TYR	88	54.566	51.093	17.734	1.00 19.03	CPS3
ATOM	2553	CG	TYR	88	53.531	51.940	18.426	1.00 19.37	CPS3
ATOM	2554	CD1		88	53.395	51.915	19.804	1.00 19.95	CPS3
ATOM	2555			88	52.413	52.683	20.449	1.00 20.13	CPS3
ATOM	2556 2557		TYR	88	52.665	52.756	17.693	1.00 19.40	CPS3
ATOM		CE2		88	51.690	53.519	18.315	1.00 19.13	CPS3
ATOM	2558 2559	CZ	TYR	88	51.562	53.479	19.691	1.00 18.55	CPS3
ATOM		ОН	TYR	88	50.568	54.204	20.299	1.00 19.71	CPS3
ATOM	2560	C	TYR	88	53.385	48.899	18.211	1.00 18.42	CPS3
ATOM	2561 2562	O N	TYR	88	52.159	48.825	18.277	1.00 18.60	CPS3
ATOM		N	ILE	89	54.196	48.233	19.020	1.00 17.79	CPS3
ATOM	2563 2564	CA CB	ILE	89	53.675	47.331	20.022	1.00 18.21	CPS3
AION	2504	CB	ILE	89	54.406	45.966	19.939	1.00 17.33	CPS3



SEP 0 9 2002

FIG. 1A-45

e e	SUBCLASS	
APPROVED D. C.	BY CLASS	RAFTSMAH

MOTA	2565	CG2	ILE	89	54.146	45.145	21.217	1.00 18.20	CPS3
ATOM	2566	CG1	ILE	89	53.938	45.192	18.696	1.00 18.54	CPS3
ATOM	2567	CD1	ILE	89	54.805	43.948	18.365	1.00 18.01	CPS3
ATOM	2568	C	ILE	89	53.775	47.829	21.450	1.00 18.41	CPS3
ATOM	2569	0	ILE	89	54.749	48.465	21.832	1.00 18.45	CPS3
ATOM	2570	N	ILE	90	52.737	47.539	22.221	1.00 19.17	CPS3
ATOM	2571	CA	ILE	90	52.722	47.852	23.645	1.00 20.34	CPS3
ATOM	2572	CB	ILE	90	51.485	48.700	24.062	1.00 21.03	CPS3
ATOM	2573		ILE	90	51.364	48.738	25.608	1.00 21.79	CPS3
ATOM	2574	CG1	ILE	90	51.605	50.128	23.516	1.00 21.75	CPS3
ATOM	2575		ILE	90	52.787	50.918	24.079	1.00 22.03	
ATOM	2576	c	ILE	90	52.618	46.483	24.314		CPS3
ATOM	2577	ō	ILE	90	51.722	45.704		1.00 20.90	CPS3
ATOM	2578	N	CYS	91	53.557	46.177	23.994	1.00 22.15	CPS3
ATOM	2579	CA	CYS	91			25.208	1.00 21.50	CPS3
ATOM	2580	CB	CYS		53.565	44.918	25.968	1.00 22.56	CPS3
ATOM	2580	SG	CYS	91	54.379	43.834	25.252	1.00 22.42	CPS3
ATOM				91	54.522	42.300	26.235	1.00 25.18	CPS3
	2582	С	CYS	91	54.251	45.307	27.279	1.00 23.27	CPS3
ATOM	2583	0	CYS	91	55.450	45.584	27.292	1.00 23.16	CPS3
ATOM	2584	N	THR	92	53.500	45.337	28.372	1.00 26.40	CPS3
ATOM	2585	CA	THR	92	54.076	45.784	29.638	1.00 28.79	CPS3
ATOM	2586	CB	THR	92	52.983	46.002	30.713	1.00 29.85	CPS3
ATOM	2587		THR	92	52.347	44.760	31.033	1.00 31.45	CPS3
ATOM	2588	CG2		92	51.934	46.993	30.195	1.00 30.30	CPS3
ATOM	2589	С	THR	92	55.203	44.945	30.217	1.00 30.27	CPS3
MOTA	2590	0	THR	92	55.787	45.313	31.237	1.00 29.37	CPS3
ATOM	2591	N	LYS	93	55.520	43.828	29.571	1.00 30.96	CPS3
ATOM	2592	CA	LYS	93	56.618	42.991	30.031	1.00 32.02	CPS3
ATOM	2593	CB	LYS	93	56.521	41.608	29.397	1.00 33.43	CPS3
ATOM	2594	CG	LYS	93	55.509	40.711	30.098	1.00 36.42	CPS3
ATOM	2595	CD	LYS	93	55.253	39.426	29.337	1.00 38.18	CPS3
ATOM	2596	CE	LYS	93	54.583	38.385	30.227	1.00 40.38	CPS3
ATOM	2597	NZ	LYS	93	53.482	38.941	31.059	1.00 41.16	CPS3
ATOM	2598	С	LYS	93	57.956	43.657	29.701	1.00 31.94	CPS3
ATOM	2599	ō	LYS	93	58.998	43.287	30.233	1.00 31.94	
ATOM	2600	N	LEU	94	57.924	44.655			CPS3
ATOM	2601	CA	LEU	94	59.139	45.378	28.824	1.00 31.18	CPS3
ATOM	2602	CB	LEU	94			28.473	1.00 30.06	CPS3
ATOM	2603	CG	LEU		59.903	44.637	27.376	1.00 31.03	CPS3
ATOM	2604		LEU	94	59.121	43.973	26.240	1.00 31.49	CPS3
ATOM	2605	CD2		94	58.228	44.977	25.551	1.00 33.11	CPS3
ATOM	2606			94	60.109	43.366	25.258	1.00 31.24	CPS3
ATOM		C	LEU	94	58.822	46.801	28.042	1.00 29.42	CPS3
	2607	0	LEU	94	57.657	47.165	27.909	1.00 28.23	CPS3
ATOM	2608	N	SER	95	59.852	47.618	27.841	1.00 28.87	CPS3
ATOM	2609	CA	SER	95	59.616	48.993	27.423	1.00 29.31	CPS3
ATOM	2610	CB	SER	95	60.853	49.867	27.631	1.00 30.92	CPS3
ATOM	2611	OG	SER	95	60.671	51.106	26.950	1.00 31.74	CPS3
MOTA	2612	С	SER	95	59.244	49.062	25.953	1.00 28.31	CPS3
ATOM	2613	0	SER	95	59.835	48.376	25.127	1.00 27.86	CPS3
ATOM	2614	N	PRO	96	58.269	49.914	25.611	1.00 28.41	CPS3
ATOM	2615	CD	PRO	96	57.504	50.793	26.516	1.00 29.30	CPS3
ATOM	2616	CA	PRO	96	57.829	50.074	24.221	1.00 27.35	CPS3
ATOM	2617	CB	PRO	96	56.749	51.155	24.312	1.00 28.52	CPS3
ATOM	2618	CG	PRO	96	56.259	51.056	25.722	1.00 29.70	CPS3
ATOM	2619	С	PRO	96	58.997	50.532	23.344	1.00 26.87	CPS3
ATOM	2620	0	PRO	96	59.060	50.332	22.156	1.00 25.42	CPS3
ATOM	2621	N	ALA	97	59.922	51.283	23.940	1.00 25.42	CPS3
					33.322	JI.283	23.940	1.00 26.21	CPS3



ATOM

2653 C VAL 101

2654 O VAL 101

2655 N SER 102

2656 CA SER 102

2657 CB SER 102

2658 OG SER 102

2659 C SER 102

2660 O SER 102

2661 N ILE 103

2662 CA

2663 CB ILE 103

2664

2665

2666

2667 C ILE 103

2668 O ILE 103

2669 N THR 104

2670 CA THR 104

2672

2673

2674 C THR 104

2675 O THR 104

2676 N HIS 105

2677 CA HIS 105

2678 CB HIS 105

2622

2623

CA ALA

CB

ALA 97

RECEIVED

SEP 0 9 2002

TECH CENTER 1600/2900

CPS3

CPS3

CPS3

CPS3

1.00 26.00

1.00 28.49

1.00 25.63

1.00 24.95

FIG. 1A-46

61.073

61.821

51.804

52.824

97

ATOM 2624 С AT.A 97 62.031 50.709 22.744 SUBCLASS ATOM 2625 0 62.858 50.921 21.858 ALA 97 ATOM 2626 N ALA 98 61.916 49.532 CA 62.793 ATOM 2627 ALA 98 48.426 ATOM 2628 CB ALA 98 63.054 47.574 C.ASS ATOM 2629 С ALA 98 62.208 47.553 ATOM 2630 0 ALA 98 62.868 46.645 ATOM N 60.979 47.842 2631 VAL 99 ATOM 2632 CA VAL 99 60.330 47.004 DRAFTSMAN ATOM 2633 CB VAL 99 58.965 46.511 ATOM 2634 CG1 VAL 99 58.383 45.474 MOTA CG2 VAL 45.930 2635 99 59.125 ATOM 2636 С VAL 99 60.100 47.691 ATOM 2637 0 VAL 99 59.758 48.865 ATOM 2638 N HIS 100 60.295 46.941 ATOM 2639 CA HIS 100 60.080 47.439 ATOM 2640 CB HIS 100 61,426 47.732 ATOM 2641 CG HIS 100 62.233 48.753 ATOM 2642 CD2 HIS 100 63.223 48.613 ATOM 2643 ND1 HIS 100 62.007 50.105 ATOM 2644 CE1 HIS 100 62.825 50.758 ATOM 2645 NE2 HIS 100 63.572 49.874 ATOM 2646 C HTS 100 59.343 46.348 ATOM 2647 0 HIS 100 59.707 45.178 ATOM 2648 N VAL 101 58.313 46.731 ATOM 2649 CA VAL 101 57.525 45.765 ATOM 2650 CB VAL 101 56.149 45.472 ATOM 2651 CG1 VAI. 101 55.316 46.753 ATOM 2652 CG2 VAL 101

ILE

THR 104

CG2 ILE

CG1 ILE

CD1 ILE

OG1 THR

CG2 THR

2671 CB

103

103

103

103

104

104

52.138

51.062

52.340

51.099

53.261

53.304

53.038

52.802

54.116

53.888

54.583

51.694

51.347

51.142

50.066

48.701 42.514

44.533

43.538

44.398

44.754

44.475

45.608

43.390

43.475

43.197

43.430

41.763

42.494

41.586

42.688

41.838

23.342 1.00 24.02 CPS3 22.986 1.00 23.40 CPS3 24.215 1.00 25.00 CPS3 21.880 1.00 22.32 CPS3 21.401 1.00 22.68 CPS3 21.460 1.00 21.24 CPS3 20.457 1.00 19.35 CPS3 20.982 1.00 19.94 CPS3 20.027 1.00 21.36 CPS3 22.376 1.00 23.27 CPS3 19.121 1.00 19.01 CPS3 19.083 1.00 19.19 CPS3 18.037 1.00 18.11 CPS3 16.685 1.00 19.23 CPS3 16.029 1.00 21.42 CPS3 16.772 1.00 24.13 CPS3 17.686 1.00 25.59 CPS3 16.654 1.00 25.95 CPS3 17.463 1.00 26.97 CPS3 18.100 1.00 26.97 CPS3 15.919 1.00 18.08 CPS3 16.027 1.00 17.62 CPS3 15.161 1.00 17.20 CPS3 14.382 1.00 16.42 CPS3 15.080 1.00 16.35 CPS3 15.156 1.00 15.91 CPS3 55.364 44.375 14.330 1.00 17.27 CPS3 57.244 46.312 12.982 1.00 16.80 CPS3 57.325 47.515 12.754 1.00 15.86 CDS3 56.948 45.414 12.046 1.00 16.94 CPS3 56.554 45.816 10.694 1.00 17.40 CPS3 57.733 45.889 9.723 1.00 18.13 CPS3 57.255 46.343 8.454 1.00 19.88 CPS3 55.566 44.752 10.240 1.00 17.06 CPS3 55.738 43.569 10.531 1.00 16.38 CPS3 54.508 45.180 9.562 1.00 16.71 CPS3 53.476 44.259 9.109 1.00 16.77 CPS3

9.851

9.386

11.366

12.195

7.615

7.140

6.880

5.438

4.636

3.246

4.822

5.020

5.770

3.825

3.320

3.515

1.00 19.32

1.00 20.27

1.00 18.63

1.00 17.98

1.00 17.09

1.00 18.12

1.00 18.52

1.00 19.66

1.00 20.60

1.00 21.77

1.00 20.35

1.00 20.81

1.00 19.47

1.00 21.19

1.00 23.77

1.00 25.55

CPS3

23.203

24.060



SEP 0 9 2002

FIG. 1A-47

2679 CG HIS 105 48.344 42.814 4.937 1.00 30.17

F1G.	SUBCLASS	
0.0	CLASS	
APPROVED	5~ 63	DRAFTSMAH

					.0.5.1	12.014	4.331	1.00 30.17	CPS3
ATOM	2680	CD2	HIS	105	48.668	43.859	5.737	1.00 31.35	CPS3
ATOM	2681	ND1	HIS	105	47.507	42.008	5.676	1.00 31.23	CPS3
ATOM	2682	CE1	HIS	105	47.327	42.544	6.872	1.00 33.22	CPS3
ATOM	2683		HIS	105	48,020	43.668	6.935	1.00 32.63	CPS3
ATOM	2684	С	HIS	105	50.178	41.619	1.817	1.00 22.69	
ATOM	2685	ō	HIS	105	50.784	42.413	1.105		CPS3
ATOM	2686	N	THR	106				1.00 22.84	CPS3
ATOM	2687	CA	THR	106	49.565	40.536	1.359	1.00 24.26	CPS3
ATOM	2688	CB	THR		49.426	40.244	-0.066	1.00 25.12	CPS3
				106	50.338	39.107	-0.598	1.00 25.65	CPS3
ATOM	2689		THR	106	49.928	37.848	-0.047	1.00 25.72	CPS3
ATOM	2690	CG2		106	51.805	39.395	-0.275	1.00 24.63	CPS3
ATOM	2691	С	THR	106	47.970	39.769	-0.097	1.00 25.84	CPS3
ATOM	2692	0	THR	106	47.290	39.753	0.934	1.00 24.47	CPS3
ATOM	2693	N	ALA	107	47.484	39.388	-1.265	1.00 25.43	CPS3
ATOM	2694	CA	ALA	107	46.108	38.937	-1.362	1.00 26.46	CPS3
ATOM	2695	CB	ALA	107	45.790	38.570	-2.820	1.00 27.17	CPS3
ATOM	2696	С	ALA	107	45.812	37.750	-0.444	1.00 26.57	CPS3
ATOM	2697	0	ALA	107	44.769	37.707	0.213	1.00 27.71	CPS3
ATOM	2698	N	GLU	108	46.738	36.799	-0.384	1.00 26.04	CPS3
ATOM	2699	CA	GLU	108	46.542	35.594	0.404	1.00 25.62	CPS3
ATOM	2700	CB	GLU	108	46.833	34.374	-0.475	1.00 29.10	
ATOM	2701	CG	GLU	108	46.172	34.475	-1.846	1.00 35.56	CPS3
ATOM	2702	CD	GLU	108	46.174	33.171	-2.616		CPS3
ATOM	2703		GLU	108	47.145	32.395		1.00 40.28	CPS3
ATOM	2704		GLU	108	45.201	32.932	-2.485	1.00 42.87	CPS3
ATOM	2705	C	GLU	108	47.325		-3.369	1.00 44.28	CPS3
ATOM	2706	ō	GLU	108		35.460	1.706	1.00 25.50	CPS3
ATOM	2707	N	TYR	109	47.087	34.520	2.463	1.00 23.92	CPS3
ATOM	2708	CA	TYR	109	48.239	36.389	1.978	1.00 23.47	CPS3
ATOM	2709				49.048	36.281	3.189	1.00 22.84	CPS3
ATOM		CB	TYR	109	50.471	35.833	2.822	1.00 23.00	CPS3
ATOM	2710	CG	TYR	109	50.552	34.480	2.176	1.00 23.82	CPS3
ATOM	2711		TYR	109	50.485	33.317	2.936	1.00 23.06	CPS3
	2712		TYR	109	50.532	32.063	2.334	1.00 24.49	CPS3
ATOM	2713		TYR	109	50.668	34.361	0.793	1.00 23.15	CPS3
ATOM	2714		TYR	109	50.710	33.122	0.184	1.00 24.59	CPS3
ATOM	2715	CZ	TYR	109	50.641	31.980	0.956	1.00 24.33	CPS3
ATOM	2716	OH	TYR	109	50.655	30.756	0.341	1.00 26.41	CPS3
ATOM	2717	С	TYR	109	49.187	37.551	4.000	1.00 21.41	CPS3
MOTA	2718	0	TYR	109	49.021	38.659	3.477	1.00 21.21	CPS3
ATOM	2719	N	ALA	110	49.478	37.366	5.293	1.00 19.67	CPS3
ATOM	2720	CA	ALA	110	49.781	38.470	6.204	1.00 19.04	CPS3
ATOM	2721	CB	ALA	110	48.753	38.588	7.334	1.00 18.93	CPS3
ATOM	2722	С	ALA	110	51.137	38.048	6.776	1.00 19.30	CPS3
ATOM	2723	0	ALA	110	51.375	36.861	6.985	1.00 20.91	CPS3
ATOM	2724	N	ALA	111	52.038	38.997	7.014	1.00 18.04	CPS3
ATOM	2725	CA	ALA	111	53.337	38.631	7.565	1.00 17.63	CPS3
ATOM	2726	CB	ALA	111	54.347	38.376	6.434	1.00 16.29	CPS3
ATOM	2727	С	ALA	111	53.819	39.758	8.469		
ATOM	2728	ō	ALA	111	53.404	40.903	8.312	1.00 17.67 1.00 18.51	CPS3
ATOM	2729	N	ALA	112	54.672				CPS3
ATOM	2730	CA	ALA	112	55.181	39.424	9.428	1.00 16.56	CPS3
ATOM	2731	CB	ALA	112		40.433	10.342	1.00 15.86	CPS3
ATOM	2732	C	ALA	112	54.203	40.636	11.489	1.00 15.01	CPS3
ATOM	2733	ō	ALA	112	56.533	40.033	10.896	1.00 17.34	CPS3
ATOM	2734	N	GLN		56.885	38.856	10.913	1.00 16.61	CPS3
ATOM	2735	CA	GLN	113	57.294	41.021	11.352	1.00 16.50	CPS3
-11011	2133	-M	GTIA	113	58.591	40.732	11.952	1.00 18.53	CPS3



SEP 0 9 2002





	SUBCLASS		1
.0.6. FIG.	CLASS SUBC		
APPROVEU	 	DRAFTSMAH	

ATOM	2736	CB	GLN	113	59.735	40.962	10.956	1.00 18.24	CPS3
ATOM	2737	CG	GLN	113	59.926	42.406	10.544	1.00 22.84	CPS3
MOTA	2738	CD	GLN	113	61.095	42.611	9.578	1.00 26.07	CPS3
ATOM	2739		GLN	113	61.504	43.738	9.326	1.00 28.00	CPS3
ATOM	2740	NE2		113	61.624	41.521	9.033	1.00 28.26	CPS3
ATOM	2741	С	GLN	113	58.724	41.667	13.144	1.00 16.72	CPS3
ATOM	2742	0	GLN	113	58.108	42.728	13.182	1.00 16.09	CPS3
ATOM	2743	N	VAL	114	59.513	41.252	14.124	1.00 17.10	CPS3
ATOM	2744	CA	VAL	114	59.707	42.051	15.329	1.00 17.04	CPS3
ATOM	2745	CB	VAL	114	58.882	41.484	16.538	1.00 17.59	CPS3
ATOM	2746		VAL	114	59.307	42.160	17.853	1.00 17.11	CPS3
ATOM	2747	CG2		114	57.392	41.703	16.320	1.00 16.91	CPS3
ATOM	2748	C	VAL	114	61.173	41.971	15.710	1.00 18.24	CPS3
ATOM	2749	0	VAL	114	61.826	40.948	15.493	1.00 16.19	CPS3
ATOM	2750	N	VAL	115	61.691	43.068	16.251	1.00 18.16	CPS3
ATOM	2751	CA	VAL	115	63.053	43.072	16.763	1.00 19.36	CPS3
ATOM	2752	CB	VAL	115	64.021	43.925	15.920	1.00 20.69	CPS3
ATOM	2753		VAL	115	65.394	44:014	16.637	1.00 20.85	CPS3
MOTA	2754	CG2		115	64.184	43.305	14.529	1.00 18.29	CPS3
ATOM	2755	С	VAL	115	62.916	43.691	18.148	1.00 20.16	CPS3
ATOM	2756	0	VAL	115	62.268	44.728	18.309	1.00 21.78	CPS3
ATOM	2757	N	ILE	116	63.463	43.018	19.152	1.00 20.33	CPS3
MOTA	2758	CA	ILE	116	63.438	43.527	20.517	1.00 21.08	CPS3
ATO:	2759	CB	ILE	116	62.911	42.491	21.517	1.00 21.66	CPS3
ATO:	2760	CG2		116	63.081	43.042	22.960	1.00 21.13	CPS3
ATOM	2761	CG1		116	61.439	42.174	21.215	1.00 21.09	CPS3
ATOM	2762	CD1		116	60.806	41.091	22.118	1.00 19.60	CPS3
ATOM	2763	С	ILE	116	64.881	43.835	20.885	1.00 24.39	CPS3
ATOM	2764	0	ILE	116	65.764	42.993	20.697	1.00 22.81	CPS3
ATOM	2765	N	GLU	117	65.131	45.041	21.381	1.00 26.58	CPS3
ATOM	2766	CA	GLU	117	66.487	45.410	21.767	1.00 31.31	CPS3
ATOM	2767	CB	GLU	117	66.824	46.834	21.346	1.00 32.50	CPS3
ATOM	2768	CG	GLU	117	66.641	47.178	19.901	1.00 37.84	CPS3
ATOM	2769	CD	GLU	117	67.052	48.616	19.638	1.00 40.98	CPS3
ATOM ATOM	2770		GLU	117	68.271	48.872	19.516	1.00 42.89	CPS3
	2771		GLU	117	66.160	49.491	19.578	1.00 43.15	CPS3
ATOM ATOM	2772	C	GLU	117	66.653	45.367	23.275	1.00 33.73	CPS3
	2773	0	GLU	117	65.679	45.454	24.026	1.00 33.05	CPS3
ATOM ATOM	2774	N	ARG	118	67.904	45.244	23.708	1.00 37.38	CPS3
ATOM	2775 2776	CA	ARG	118	68.224	45.267	25.124	1.00 41.10	CPS3
ATOM	2777	CB CG	ARG	118	69.512	44.496	25.407	1.00 42.40	CPS3
ATOM	2778	CD	ARG	118	69.311	43.126	26.025	1.00 44.67	CPS3
ATOM	2779		ARG	118	70.649	42.566	26.483	1.00 45.83	CPS3
ATOM	2780	NE CZ	ARG	118	71.614	42.542	25.389	1.00 47.03	CPS3
ATOM	2781	NH1	ARG	118	71.609	41.652	24.402	1.00 47.03	CPS3
ATOM	2782	NH2		118	70.690	40.694	24.367	1.00 46.54	CPS3
ATOM	2783	C	ARG	118	72.520	41.729	23.446	1.00 46.88	CPS3
ATOM	2784	0	ARG	118	68.452	46.744	25.399	1.00 42.76	CPS3
ATOM	2785	N		118	69.227	47.392	24.697	1.00 44.45	CPS3
ATOM	2786	CA	LEU	119	67.765	47.289	26.392	1.00 45.54	CPS3
ATOM	2787	· CB	LEU	119	67.928	48.699	26.722	1.00 47.93	CPS3
ATOM	2788	CG	LEU	119	66.563	49.328	27.014	1.00 48.16	CPS3
ATOM	2789	CD1		119	65.944	50.257	25.963	1.00 47.88	CPS3
ATOM	2790	CD2		119	66.182	49.739	24.548	1.00 47.81	CPS3
ATOM	2791	CD2	LEU	119	64.460	50.385	26.260	1.00 47.26	CP\$3
ATOM	2792	OT1		119 119	68.845	48.862	27.928	1.00 49.49	CPS3
		511	~50	119	70.001	49.296	27.728	1.00 50.38	CPS3



SEP 0 9 2002

FIG. 1A-49

	SUBCLASS	٦
0.6. FIG.	C. ASS SUBC	-
APPROVED	 	DRAFTSMAN

ATOM	2793		LEU	119	68.399	48.537	29.052	1.00 51.04	CPS3
MOTA	2794	С	GLY	0	33.524	21.933	24.405	1.00 41.93	CPS4
MOTA	2795	0	GLY	0	33.109	21.427	23.356	1.00 43.93	CPS4
MOTA	2796	N	GLY	0	35.967	22.519	24.212	1.00 43.67	CPS4
ATOM	2797	CA	GLY	0	34.574	23.033	24.374	1.00 42.80	CPS4
MOTA	2798	N	GLY	1	33.089	21.565	25.607	1.00 38.91	CPS4
MOTA	2799	CA	GLY	1	32.082	20.530	25.746	1.00 34.29	CPS4
ATOM	2800	С	GLY	1	30.697	21.104	25.995	1.00 31.42	CPS4
ATOM	2801	0	GLY	1	29.713	20.369	26.051	1.00 30.75	CPS4
ATOM	2802	N	ILE	2	30.618	22.419	26.172	1.00 28.92	CPS4
ATOM	2803	CA	ILE	2	29.328	23.068	26.405	1.00 26.32	CPS4
ATOM	2804	CB	ILE	2	29.309	23.809	27.765	1.00 26.73	CPS4
ATOM	2805	CG2	ILE	2	28.044	24.683	27.891	1.00 24.71	CPS4
ATOM	2806	CG1	ILE	2	29.358	22.779	28.896	1.00 27.21	CPS4
ATOM	2807	CD1	ILE	2	29.417	23.387	30.265	1.00 28.66	CPS4
ATOM	2808	С	ILE	2	29.028	24.043	25.277	1.00 25.17	CPS4
ATOM	2809	0	ILE	2	29.861	24.874	24.922	1.00 24.41	CPS4
ATOM	2810	N	TYR	3	27.839	23.910	24.703	1.00 24.67	CPS4
ATOM	2811	CA	TYR	3	27.389	24.765	23.606	1.00 24.61	CPS4
ATOM	2812	CB	TYR	3	26.260	24.071	22.850	1.00 27.01	CPS4
ATOM	2813	CG	TYR	3	25.726	24.865	21.681	1.00 29.25	CPS4
ATOM	2814	CD1	TYR	3	26.385	24.861	20.452	1.00 31.33	CPS4
ATOM	2815	CE1	TYR	3	25.916	25.616	19.379	1.00 33.16	CPS4
ATOM	2816	CD2	TYR	3	24.579	25.645	21.811	1.00 31.21	CPS4
ATOM	2817	CE2	TYR	3	24.101	26.409	20.740	1.00 32.57	CPS4
ATOM	2818	CZ	TYR	3	24.776	26.388	19.530	1.00 34.44	CPS4
ATOM	2819	OH	TYR	3	24.328	27.148	18.473	1.00 36.34	CPS4
ATOM	2820	С	TYR	3	26.881	26.103	24.151	1.00 23.47	CPS4
ATOM	2821	0	TYR	3	27.167	27.175	23.609	1.00 22.30	CPS4
ATOM	2822	N	GLY	4	26.111	26.036	25.226	1.00 21.50	CPS4
ATOM	2823	CA	GLY	4	25.597	27.262	25.802	1.00 20.66	CPS4
ATOM	2824	С	GLY	4	24.775	26.974	27.036	1.00 18.15	CPS4
ATOM	2825	0	GLY	4	24.397		27.275	1.00 17.40	CPS4
ATOM	2826	N	ILE	5	24.519	28.019	27.827	1.00 17.22	CPS4
ATOM	2827	CA	ILE	5	23.725	27.874	29.039	1.00 16.89	CPS4
ATOM	2828	CB	ILE	5	24.585	27.961	30.311	1.00 17.48	CPS4
ATOM	2829	CG2	ILE	5	25.700	26.921	30.241	1.00 16.93	CPS4
ATOM	2830	CG1	ILE	5	25.166	29.374	30.472	1.00 18.44	CPS4
ATOM	2831		ILE	5	26.002	29.560	31.716	1.00 17.67	CPS4
ATOM	2832	C	ILE	5	22.673	28.972	29.079	1.00 16.76	CPS4
ATOM	2833	0	ILE	5	22.831	30.024	28.457	1.00 17.03	CPS4
ATOM	2834	N	GLY	6	21.601	28.723	29.816	1.00 16.72	CPS4
ATOM	2835	CA	GLY	6	20.537	29.702	29.894	1.00 17.09	CPS4
ATOM	2836	С	GLY	6	19.874	29.687	31.246	1.00 17.29	CPS4
ATOM	2837	0	GLY	6	19.730	28.638	31.869	1.00 17.78	CPS4
ATOM	2838	N	LEU	7	19.485	30.874	31.703	1.00 16.88	CPS4
ATOM	2839	CA	LEU	7	18.825	31.033	32.990	1.00 17.08	CPS4
ATOM	2840	CB	LEU	7	19.803	31.622	34.006	1.00 17.08	CPS4
ATOM	2841	CG	LEU	7	19.251	31.984	35.389	1.00 18.23	CPS4
ATOM	2842		LEU	7	18.988	30.707	36.200	1.00 17.58	CPS4
ATOM	2843		LEU	7	20.282	32.875	36.200	1.00 17.38	. CPS4
ATOM	2844	c	LEU	7	17.660	31.998		1.00 17.74	CPS4
ATOM	2845	ō	LEU	7	17.775	32.976	32.817 32.082	1.00 18.06	CPS4
ATOM	2846	N	ASP	8	16.539				
ATOM	2847	CA	ASP	8	15.394	31.712	33.471		CPS4
ATOM	2848	СВ	ASP	8	14.426	32.612	33.413	1.00 18.03 1.00 20.37	CPS4 CPS4
ATOM	2849	CG	ASP	8		32.202	32.305		
				٠	13.195	33.108	32.250	1.00 22.41	CPS4



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TECH CENTER 1600/2900

FIG. 1A-50

APPROVED 1 D. F. IG.
EY GLASS SUBCLASS
DRATISMAN

ATOM	2850	OD1	ASP	8	12.194	32.814	32.922	1.00 25.67	CPS4
ATOM	2851		ASP	8	13.245	34.131	31.551	1.00 24.39	CPS4
ATOM	2852	C	ASP	8	14.645	32.619	34.732	1.00 19.46	CPS4
ATOM	2853	0	ASP	8	14.490	31.574			
		N					35.363	1.00 17.36	CPS4
ATOM	2854		ILE	9	14.239	33.806	35.183	1.00 18.34	CPS4
ATOM	2855	CA	ILE	9	13.420	33.898	36.376	1.00 19.60	CPS4
ATOM	2856	CB	ILE	9	14.086	34.711	37.519	1.00 19.76	CPS4
ATOM	2857		ILE	9	13.133	34.805	3 8.7 00	1.00 21.48	CPS4
ATOM	2858	CG1	ILE	9	15.366	34.012	37.982	1.00 20.86	CPS4
ATOM	2859	CD1	ILE	9	16.146	34.790	39.050	1.00 22.16	CPS4
ATOM	2860	С	ILE	9	12.171	34.623	35.878	1.00 20.38	CPS4
ATOM	2861	0	ILE	9	12.277	35.629	35.167	1.00 20.64	CPS4
ATOM	2862	N	THR	10	10.996	34.086	36.205	1.00 19.99	CPS4
ATOM	2863	CA	THR	10	9.749	34.700	35.781	1.00 20.69	CPS4
ATOM	2864	CB	THR	10	8.999	33.803	34.777	1.00 21.55	CPS4
ATOM	2865		THR	10	9.775	33.679	33.572	1.00 23.30	CPS4
ATOM	2866	CG2		10	7.639	34.414			
ATOM	2867	C	THR	10			34.433	1.00 23.59	CPS4
ATOM					8.833	34.990	36.970	1.00 20.24	CPS4
	2868	0	THR	10	8.677	34.166	37.865	1.00 18.97	CPS4
ATOM	2869	N	GLU	11	8.233	36.173	36.971	1.00 21.51	CPS4
ATOM	2870	CA	GLU	11	7.321	36.560	38.045	1.00 23.43	CPS4
ATOM	2871	CB	GLU	11	7.180	38.085	38.070	1.00 26.54	CPS4
ATOM	2872	CG	GLU	11	6.189	38.601	39.095	1.00 28.77	CPS4
ATOM	2873	CD	GLU	11	6.072	40.116	39.097	1.00 30.52	CPS4
ATOM	2874	OE1	GLU	11	6.416	40.744	38.078	1.00 29.88	CPS4
ATOM	2875	OE2	GLU	11	5.615	40.675	40.118	1.00 33.84	CPS4
ATOM	2876	С	GLU	11	5.959	35.906	37.791	1.00 24.01	CPS4
ATOM	2877	0	GLU	11	5.344	36.137	36.750	1.00 23.79	CPS4
ATOM	2878	N	LEU	12	5.482	35.092	38.730	1.00 23.66	CPS4
ATOM	2879	CA	LEU	12	4.191	34.416	38.556	1.00 25.00	CPS4
ATOM	2880	CB	LEU	12	3.804	33.609	39.798	1.00 25.00	CPS4
ATOM	2881	CG	LEU	12	4.621	32.386	40.208	1.00 28.31	
ATOM	2882		LEU	12	3.877				CPS4
ATOM	2883		LEU	12		31.679	41.347	1.00 31.83	CPS4
ATOM	2884	CD2			4.808	31.435	39.028	1.00 32.20	CPS4
ATOM			LEU	12	3.044	35.391	38.253	1.00 24.98	CPS4
	2885	0	LEU	12	2.196	35.107	37.412	1.00 24.51	CPS4
ATOM	2886	N	ALA	13	3.019	36.524	38.950	1.00 25.40	CPS4
ATOM	2887	CA	ALA	13	1.968	37.527	38.744	1.00 25.67	CPS4
ATOM	2888	CB	ALA	13	2.157	38.691	39.702	1.00 28.52	CPS4
ATOM	2889	C	ALA	13	1.939	38.044	37.314	1.00 26.33	CPS4
ATOM	2890	0	ALA	13	0.871	38.344	36.781	1.00 26.54	CPS4
ATOM	2891	N	ARG	14	3.107	38.152	36.688	1.00 24.68	CPS4
ATOM	2892	CA	ARG	14	3.179	38.644	35.318	1.00 26.32	CPS4
ATOM	2893	CB	ARG	14	4.644	38.886	34.925	1.00 28.73	CPS4
ATOM	2894	CG	ARG	14	4.859	39.331	33.482	1.00 34.36	CPS4
ATOM	2895	CD	ARG	14	6.328	39.142	33.058	1.00 37.57	CPS4
ATOM	2896	NE	ARG	14	6.497	39.219	31.608	1.00 37.37	CPS4
ATOM	2897	CZ	ARG	14	7.529	38.704			
ATOM	2898	NH1		14			30.947	1.00 42.56	CPS4
ATOM	2899	NH2			8.491	38.070	31.603	1.00 43.08	CPS4
ATOM	2900			14	7.597	38.817	29.627	1.00 44.77	CPS4
ATOM		c	ARG	14	2.533	37.633	34.370	1.00 25.53	CPS4
	2901	0	ARG	14	1.783	38.001	33.465	1.00 25.68	CPS4
ATOM	2902	N	ILE	15	2.832	36.357	34.585	1.00 24.70	CPS4
ATOM	2903	CA	ILE	15	2.278	35.284	33.763	1.00 25.07	CPS4
ATOM	2904	CB	ILE	15	2.884	33.920	34.153	1.00 24.95	CPS4
ATOM	2905	CG2		15	2.169	32.782	33.390	1.00 24.82	CPS4
ATOM	2906	CG1	ILE	15	4.382	33.913	33.849	1.00 24.68	CPS4



SEP 0 9 2002 TECH CENTER 1600/2900

100	ATOM	2909	0
3. BCLASS	ATOM	2910	N
1 .15 1	ATOM	2911	CA
	ATOM	2912	CB
14 60	ATOM	2913	C
10:18	ATOM	2914	0
1315 1	ATOM	2915	N
1212	ATOM	2916	CA
APPROVED EY RAFTSHAM	ATOM	2917	CB
APPROVE EY ORAFISHAN	ATOM	2918	OG
E =	ATOM	2919	С
8	ATOM	2920	0
	ATOM	2921	N
	ATOM	2922	CA
	ATOM	2923	CB
	ATOM	2924	CG
	ATOM	2925	SD
	ATOM	2926	CE
	ATOM	2927	С
	ATOM	2928	0

ATOM	2907		ILE	15	4.714	33.980	32.358	1.00 27.32	CPS4
ATOM	2908	С	ILE	15	0.766	35,200	33.950	1.00 26.73	CPS4
ATOM	2909	0	ILE	15	0.009	34.983	32.993	1.00 25.85	CPS4
ATOM	2910	N	ALA	16	0.324	35.352	35.193	1.00 26.46	CPS4
ATOM	2911	CA	ALA	16	-1.104	35.273	35.469	1.00 27.92	CPS4
ATOM	2912	CB	ALA	16	-1.355	35.318	36.975	1.00 28.33	CPS4
ATOM	2913	С	ALA	16	-1.823	36.423	34.774	1.00 29.55	CPS4
ATOM	2914	0	ALA	16	-2.928	36.252	34.240	1.00 29.47	CPS4
ATOM	2915	N	SER	17	-1.191	37.592	34.772	1.00 29.18	CPS4
ATOM	2916	CA	SER	17	-1.783	38.760	34.136	1.00 31.51	CPS4
ATOM	2917	CB	SER	17	-0.944	40.000	34.429	1.00 33.05	CPS4
ATOM	2918	OG	SER	17	-1.421	41.104	33.672	1.00 39.63	CPS4
ATOM	2919	C	SER	17	-1.922	38.574	32.624	1.00 32.08	CPS4
ATOM	2920	0	SER	17	-2.974	38.874	32.045	1.00 31.35	CPS4
ATOM	2921	N	MET	18	-0.871	38.078	31.982	1.00 31.52	CPS4
ATOM	2922	CA	MET	18	-0.912	37.868	30.540	1.00 32.75	CPS4
ATOM	2923	CB	MET	18	0.469	37.482	30.008	1.00 34.03	CPS4
ATOM	2924	CG	MET	18	1.504	38.580	30.147	1.00 38.00	CPS4
ATOM	2925	SD	MET	18	3.076	38.170	29.360	1.00 41,64	CPS4
ATOM	2926	CE	MET	18	3.866	37.225	30.666	1.00 38.75	CPS4
ATOM	2927	С	MET	18	-1.917	36.793	30.156	1.00 32.75	CPS4
ATOM	2928	0	MET	18	-2.689	36.971	29.215	1.00 32.74	CPS4
MOTA	2929	N	ALA	19	-1.906	35.686	30.893	1.00 33.01	CPS4
ATOM	2930	CA	ALA	19	-2.801	34.569	30.618	1.00 34.57	CPS4
ATOM	2931	CB	ALA	19	-2.458	33.384	31.515	1.00 34.76	CPS4
ATOM	2932	,C	ALA	19	-4.262	34.944	30.793	1.00 36.04	CPS4
ATOM	2933	0	ALA	19	-5.140	34.338	30.176	1.00 36.08	CPS4
ATOM	2934	N	GLY	20	-4.523	35.942	31.630	1.00 36.62	CPS4
ATOM	2935	CA	GLY	20	-5.896	36.360	31.852	1.00 38.42	CPS4
MOTA	2936	С	GLY	20	-6.379	37.392	30.850	1.00 38.57	CPS4
ATOM	2937	0	GLY	20	-7.560	37.437	30.511	1.00 38.87	CPS4
MOTA	2938	N	ARG	21	-5.460	38.210	30.355	1.00 38.64	CPS4
ATOM	2939	CA	ARG	21	-5.813	39.261	29.417	1.00 39.87	CPS4
ATOM	2940	CB	ARG	21	-4.944	40.489	29.695	1.00 42.18	CPS4
MOTA	2941	CG	ARG	21	-4.955	40.913	31.156	1.00 47.12	CPS4
ATOM	2942	CD	ARG	21	-4.162	42.195	31.381	1.00 50.94	CPS4
ATOM	2943	NE	ARG	21	-4.149	42.582	32.792	1.00 55.15	CPS4
ATOM	2944	CZ	ARG	21	-3.691	43.746	33.252	1.00 56.93	CPS4
ATOM	2945	NH1	ARG	21	-3.721	44.005	34.554	1.00 57.41	CPS4
ATOM	2946	NH2	ARG	21	-3.211	44.656	32.412	1.00 57.54	CPS4
ATOM	2947	С	ARG	21	-5.699	38.879	27.942	1.00 39.28	CPS4
ATOM	2948	0	ARG	21	-6.223	39.587	27.080	1.00 39.05	CPS4
ATOM	2949	N	GLN	22	-5.030	37.764	27.655	1.00 37.77	CPS4
ATOM	2950	CA	GLN	22	-4.823	37.311	26.276	1.00 37.67	CPS4
ATOM	2951	CB	GLN	22	-3.325	37.254	25.979	1.00 36.76	CPS4
ATOM	2952	CG	GLN	22	-2.634	38.603	26.038	1.00 40.23	CPS4
ATOM	2953	CD	GLN	22	-1.135	38.490	25.871	1.00 41.78	CPS4
ATOM	2954	OE1	GLN	22	-0.652	37.746	25.018	1.00 43.79	CPS4
ATOM	2955	NE2	GLN	22	-0.389	39.236	26.677	1.00 42.68	CPS4
ATOM	2956	С	GLN	22	-5.441	35.947	25.997	1.00 37.08	CPS4
MOTA	2957	0	GLN	22	-5.004	34.936	26.560	1.00 37.84	CPS4
ATOM	2958	N	LYS	23	-6.431	35.910	25.106	1.00 34.80	CPS4
ATOM	2959	CA	LYS	23	-7.114	34.661	24.781	1.00 34.70	CPS4
ATOM	2960	CB	LYS	23	-8.133	34.862	23.641	1.00 35.14	CPS4
ATOM	2961	CG	LYS	23	-9.497	35.362	24.090	1.00 37.14	CPS4
ATOM	2962	CD	LYS	23	-10.626	34.901	23.159	1.00 37.14	CPS4
ATOM	2963	CE	LYS	23	-10.491	35.444	21.745	1.00 36.38	CPS4
							-1.743		C. 54

SEP 0 9 2002

TECH CENTER 1600/2900



-	1	
1.	SUBCLASS	
FIG	1	_
0.6.	CLASS	
APPROVED		TSWAH
APP	•3	DRAFTSMA

ATOM	2964	NZ	LYS	23	-11.732	35.177	20.937	1.00 32.97	CPS4
ATOM	2965	С	LYS	23	-6.211	33.491	24.403	1.00 32,65	CPS4
ATOM	2966	0	LYS	23	-6.488	32.356	24.775	1.00 33.18	CPS4
ATOM	2967	N	ARG	24	-5.143	33.754	23.659	1.00 31.45	CPS4
ATOM	2968	CA	ARG	24	-4.265	32.662	23.227	1.00 31.24	CPS4
MOTA	2969	CB	ARG	24	-4.159	32.665	21.691	1.00 32.20	CPS4
ATOM	2970	CG	ARG	24	-5.218	31.798	20.979	1.00 34.37	CPS4
ATOM	2971	CD	ARG	24	-6.636	32.172	21.379	1.00 34.60	CPS4
ATOM	2972	NE	ARG	24	-7.668	31.404	20.672	1.00 34.87	CPS4
ATOM	2973	CZ	ARG	24	-8.339	30.379	21.191	1.00 34.53	CPS4
ATOM	2974		ARG	24	-8.095	29.976	22.428	1.00 33.25	CPS4
ATOM	2975		ARG	24	-9.281	29.770	20.478	1.00 35.11	CPS4
ATOM	2976	C	ARG	24	-2.864	32.603	23.832	1.00 29.23	CPS4
ATOM	2977	ō	ARG	24	-1.967	31.992	23.259	1.00 28.10	CPS4
ATOM	2978	N	PHE	25	-2.669	33.208	24.995	1.00 27.93	CPS4
ATOM	2979	CA	PHE	25	-1.339	33.186	25.604	1.00 26.76	CPS4
ATOM	2980	CB	PHE	25	-1.339	33.979	26.916	1.00 27.25	CPS4
ATOM	2981	CG	PHE	25	0.016	34.068	27.564	1.00 28.14	CPS4
ATOM	2982		PHE	25	0.301	33.345	28.716	1.00 29.02	CPS4
ATOM	2983	CD2		25	1.023	34.837	26.986	1.00 29.76	CPS4
ATOM	2984		PHE	25	1.576	33.380	29.286	1.00 29.84	CPS4
ATOM	2985	CE2		25	2,304	34.879	27.547	1.00 31.14	CPS4
MOTA	2986	CZ	PHE	25	2.579	34.146	28.699	1.00 28.80	CPS4
ATOM	2987	C	PHE	25	-0.822	31.763	25.857	1.00 24.98	CPS4
ATOM	2988	ō	PHE	25	0.244	31.385	25.364	1.00 25.69	CPS4
ATOM	2989	N	ALA	26	-1.569	30.979	26.627	1.00 23.55	CPS4
ATOM	2990	CA	ALA	26	-1.158	29.609	26.932	1.00 23.50	CPS4
ATOM	2991	CB	ALA	26	-2.187	28.935	27.812	1.00 23.29	CPS4
ATOM	2992	c	ALA	26	-0.968	28.785	25.668	1.00 23.71	CPS4
ATOM	2993	0	ALA	26	-0.022	27.999	25.567	1.00 22.90	CPS4
ATOM	2994	N	GLU	27	-1.887	28.951	24.719	1.00 23.56	CPS4
MOTA	2995	CA	GLU	27	-1.837	28.211	23.460	1.00 23.91	CPS4
ATOM	2996	CB	GLU	27	-3.114	28.471	22.645	1.00 25.46	CPS4
ATOM	2997	CG	GLU	2 7	-4.387	27.805	23.184	1.00 28.50	CPS4
ATOM	2998	CD	GLU	27	-4.892	28.403	24.499	1.00 32.43	CPS4
ATOM	2999		GLU	27	-4.603	29.589	24.774	1.00 31.29	CPS4
ATOM	3000		GLU	27	-5.589	27.682	25.255	1.00 33.07	CPS4
ATOM	3001	С	GLU	27	-0.610	28.550	22.615	1.00 23.66	CPS4
ATOM	3002	ō	GLU	27	-0.152	27.734	21.822	1.00 24.71	CPS4
ATOM	3003	N	ARG	28	-0.081	29.754	22.779	1.00 24.04	CPS4
ATOM	3004	CA	ARG	28	1.094	30.170	22.016	1.00 25.19	CPS4
ATOM	3005	CB	ARG	28	1.191	31.696	22.047	1.00 28.07	CPS4
MOTA	3006	CG	ARG	28	1.800	32.351	20.829	1.00 33.41	CPS4
ATOM	3007	CD	ARG	28	0.994	33.602	20.446	1.00 34.25	CPS4
ATOM	3008	NE	ARG	28	0.767	34.484	21.592	1.00 35.45	CPS4
ATOM	3009	CZ	ARG	28	-0.389	35.097	21.853	1.00 37.30	CPS4
ATOM	3010		ARG	28	-1.433	34.929	21.050	1.00 35.32	CPS4
ATOM	3011		ARG	28	-0.506	35.871	22.928	1.00 37.39	CPS4
ATOM	3012	С	ARG	28	2.355	29.564	22.634	1.00 24.51	CPS4
ATOM	3013	ō	ARG	28	3.295	29.188	21.933	1.00 23.41	CPS4
ATOM	3014	N	ILE	29	2.348	29.459	23.956	1.00 22.84	CPS4
ATOM	3015	CA	ILE	29	3.498	28.959	24.707	1.00 23.13	CPS4
ATOM	3016	CB	ILE	29	3.462	29.482	26.175	1.00 24.30	CPS4
ATOM	3017	CG2	ILE	29	4.666	28.961	26.957	1.00 24.45	CPS4
ATOM	3018		ILE	29	3.390	31.014	26.192	1.00 25.98	CPS4
ATOM	3019		ILE	29	4.519	31.704	25.507	1.00 27.67	CPS4
ATOM	3020	c	ILE	29	3.628	27.450	24.787	1.00 27.56	CPS4



SEP 0 9 2002

FIG. 1A-53



ATOM	3021	0	ILE	29	4.739	26.914	24.700	1.00 22.11	CPS4
ATOM	3022	N	LEU	30	2.492	26.774	24.952	1.00 20.94	CPS4
MOTA	3023	CA	LEU	30	2.456	25.334	25.150	1.00 20.47	CPS4
MOTA	3024	CB	LEU	30	1.447	25.009	26.264	1.00 20.33	CPS4
ATOM	3025	CG	LEU	30	1.660	25.741	27.600	1.00 23.00	CPS4
ATOM	3026		LEU	30	0.511	25.425	28.561	1.00 23.25	CPS4
ATOM	3027	CD:		30	2.999	25.331	28.199	1.00 20.84	CPS4
ATOM	3028	С	LEU	30	2.120	24.493	23.936	1.00 21.35	CPS4
ATOM	3029	0	LEU	30	1.279	24.870	23.127	1.00 22.16	CPS4
MOTA	3030	N	THR	31	2.781	23.344	23.821	1.00 21.39	CPS4
ATOM	3031	CA	THR	31	2.505	22.428	22.727	1.00 22.79	CPS4
ATOM	3032	CB	THR	31	3.594	21.347	22.587	1.00 23.24	CPS4
ATOM	3033	OG 1	THR	31	3.631	20.550	23.778	1.00 24.29	CPS4
ATOM	3034	CG2	THR	31	4.960	21.996	22.356	1.00 24.52	CPS4
MOTA	3035	C	THR	31	1.186	21.736	23.052	1.00 25.13	CPS4
MOTA	3036	0	THR	31	0.646	21.868	24.158	1.00 24.76	CPS4
MOTA	3037	N	ARG	32	0.672	20.974	22.096	1.00 27.56	CPS4
ATOM	3038	CA	ARG	32	-0.594	20.289	22.298	1.00 30.79	CPS4
ATOM	3039	CB	ARG	32	-0.951	19.489	21.041	1.00 33.62	CPS4
ATOM	3040	CG	ARG	32	-2.328	19.807	20.476	1.00 38.29	CPS4
ATOM	3041	CD	ARG	32	-3.419	18.876	21.014	1.00 42.11	CPS4
ATOM	3042	NE	ARG	32	-4.044	19.329	22.259	1.00 45.08	CPS4
MOTA	3043	CZ	ARG	32	-4.676	20.491	22.409	1.00 46.06	CPS4
ATOM	3044	NH1	ARG	32	-4.774	21.348	21.393	1.00 45.64	CPS4
ATOM	3045	NH2	ARG	32	-5.224	20.792	23.577	1.00 45.73	CPS4
ATOM	3046	С	ARG	32	-0.577	19.384	23.524	1.00 30.10	CPS4
ATOM	3047	0	ARG	32	-1.527	19.388	24.310	1.00 30.78	CPS4
MOTA	3048	N	SER	33	0.499	18.620	23.699	1.00 30.30	CPS4
ATOM	3049	CA	SER	33	0.615	17.722	24.850	1.00 30.30	CPS4
ATOM	3050	CB	SER	33	1.853	16.833	24.715	1.00 32.43	CPS4
ATOM	3051	OG	SER	33	1.709	15.944	23.620	1.00 37.42	CPS4
MOTA	3052	C	SER	33	0.684	18.489	26.168	1.00 37.42	CPS4
ATOM	3053	0	SER	33	0.054	18.108	27.153	1.00 31.00	CPS4
MOTA	3054	N	GLU	34	1.464	19.564	26.191	1.00 28.83	CPS4
MOTA	3 055	CA	GLU	34	1.589	20.370	27.400	1.00 27.36	CPS4
MOTA	3056	CB	GLU	34	2.621	21.487	27.192	1.00 26.46	CPS4
ATOM	3057	CG	GLU	34	4.048	20.963	27.099	1.00 24.49	CPS4
MOTA	3058	CD	GLU	34	5.074	22.029	26.712	1.00 24.80	CPS4
ATOM	3059	OE1	GLU	34	6.223	21.934	27.196	1.00 23.27	CPS4
ATOM	3060	OE2	GLU	34	4.748	22.943	25.920	1.00 23.27	CPS4
ATOM	3061	С	GLU	34	0.232	20.962	27.757	1.00 27.85	CPS4
MOTA	3062	0	GLU	34	-0.138	21.028	28.928	1.00 27.48	CPS4
ATOM	3063	N	LEU	35	-0.513	21.392	26.742	1.00 27.48	CPS4
ATOM	3064	CA	LEU	35	-1.840	21.960	26.968	1.00 29.32	CPS4
MOTA	3065	CB	LEU	35	-2.428	22.478	25.657	1.00 27.71	CPS4
ATOM	3066	CG	LEU	35	-1.986	23.882	25.261	1.00 28.10	CPS4
ATOM	3067	CD1	LEU	35	-2.379	24.130	23.810	1.00 28.81	CPS4
ATOM	3068	CD2	LEU	35	-2.629	24.928	26.202	1.00 25.30	CPS4
ATOM	3069	С	LEU	35	-2.782	20.931	27.572	1.00 30.93	CPS4
ATOM	3070	0	LEU	35	-3.617	21.263	28.417	1.00 30.33	CPS4
ATOM	3071	N	ASP	36	-2.659	19.681	27.135	1.00 31.38	CPS4
ATOM	3072	CA	ASP	36	-3.513	18.632	27.135	1.00 33.94	CPS4
ATOM	3073	CB	ASP	36	-3.206	17.274	27.673	1.00 35.97	CPS4
ATOM	3074	CG	ASP	36	-3.763	17.156	25.612	1.00 37.70	CPS4
ATOM	3075	OD1	ASP	36	-4.838	17.727	25.812	1.00 39.64	
ATOM	3076		ASP	36	-3.134	16.475	25.332	1.00 41.16	CPS4
ATOM	3077	c	ASP	36	-3.134	18.560			
					-3.306	10.300	29.182	1.00 36.01	CPS4



SEP 0 9 2002

FIG. 1A-54



ATOM	3078	0	ASP	36	-4.269	18.440	29.933	1.00 36.88	CPS4
ATOM	3079	N	GLN	37	-2.054	18.645	29.626	1.00 35.23	CPS4
ATOM	3080	CA	GLN	37	-1.750	18.612	31.057	1.00 34.91	CPS4
ATOM	3081	CB	GLN	37	-0.238	18.552	31.278	1.00 36,27	CPS4
MOTA	3082	CG	GLN	37	0.417	17.271	30.798	1.00 40.16	CPS4
MOTA	3083	CD	GLN	. 37	1.925	17.394	30.676	1.00 41.54	CPS4
ATOM	3084	OE	GLN	37	2.436	18.146	29.845	1.00 42.68	CPS4
ATOM	3085	NE2	GLN	37	2.647	16.656	31.509	1.00 43.46	CPS4
ATOM	3086	C	GLN	37	-2.302	19.869	31.722	1.00 33.96	CPS4
MOTA	3087	0	GLN	37	-2.985	19.810	32.743	1.00 33.94	CPS4
ATOM	3088	N	TYR	38	-1.990	21.009	31.120	1.00 32.47	CPS4
ATOM	3089	CA	TYR	38	-2.422	22.315	31.601	1.00 31.95	CPS4
ATOM	3090	CB	TYR	38	-1.938	23.378	30.617	1.00 30.34	CPS4
ATOM	3091	CG	TYR	38	-2.442	24.776	30.869	1.00 29.96	CPS4
MOTA	3092	CD1	TYR	38	-3.488	25.308	30.110	1.00 30.42	CPS4
MOTA	3093	CE1		38	-3.905	26.618	30.287	1.00 30.73	CPS4
ATOM	3094	CD2		38	-1.836	25.593	31.821	1.00 28.80	CPS4
ATOM	3095	CE2	TYR	38	-2.248	26.906	32.005	1.00 29.56	CPS4
MOTA	3096	CZ	TYR	38	-3.278	27.411	31.238	1.00 31.46	CPS4
ATOM	3097	OH	TYR	38	-3.689	28.710	31.428	1.00 32.91	CPS4
ATOM	3098	C	TYR	38	-3.936	22.438	31.803	1.00 32.87	CPS4
ATOM	3099	0	TYR	38	-4.388	22.888	32.854	1.00 31.90	CPS4
MOTA	3100	N	TYR	39	-4.716	22.040	30.801	1.00 34.25	CPS4
ATOM	3101	CA	TYR	39	-6.167	22.151	30.905	1.00 36.14	CPS4
ATOM	3102	CB	TYR	39	-6.842	21.687	29.605	1.00 36.53	CPS4
ATOM	3103	CG	TYR	39	-6.618	22.577	28.390	1.00 36.61	CPS4
ATOM	3104	CD1		39	-6.608	23.970	28.504	1.00 36.59	CPS4
ATOM	3105	CE1		39	-6.471	24.791	27.378	1.00 37.06	CPS4
ATOM	3106	CD2		39	-6.483	22.021	27.115	1.00 36.55	CPS4
ATOM	3107	CE2		39	-6.347	22.830	25.980	1.00 37.48	CPS4
ATOM	3108	CZ	TYR	39	-6.343	24.213	26.118	1.00 37.69	CPS4
ATOM	3109	OH	TYR	39	-6.224	25.011	24.998	1.00 37.54	CPS4
ATOM	3110	С	TYR	39	-6.734	21.354	32.080	1.00 37.42	CPS4
ATOM	3111	0	TYR	39	-7.809	21.667	32.584	1.00 38.66	CPS4
ATOM	3112	N	GLU	40	-6.010	20.334	32.524	1.00 39.15	CPS4
ATOM	3113	CA	GLU	40	-6.476	19.491	33.622	1.00 41.54	CPS4
MOTA	3114	CB	GLU	40	-5.862	18.094	33.502	1.00 43.99	CPS4
ATOM	3115	CG	GLU	40	-6.257	17.341	32.235	1.00 48.54	CPS4
ATOM	3116	CD	GLU	40	-7.761	17.149	32.111	1.00 50.97	CPS4
ATOM	3117		GLU	40	-8.377	16.647	33.076	1.00 53.41	CPS4
ATOM	3118		GLU	40	-8.329	17.495	31.050	1.00 52.53	CPS4
ATOM	3119	C	GLU	40	-6.181	20.035	35.009	1.00 41.32	CPS4
ATOM	3120	0	GLU	40	-6.687	19.516	36.006	1.00 41.95	CPS4
ATOM	3121	N	LEU	41	-5.374	21.085	35.075	1.00 40.03	CPS4
ATOM	3122	CA	LEU	41	-4.988	21.666	36.353	1.00 38.83	CPS4
ATOM	3123	CB	LEU	41	-3.589	22.283	36.230	1.00 37.58	CPS4
ATOM	3124	CG	LEU	41	-2.457	21.303	35.908	1.00 36.93	CPS4
ATOM	3125		LEU	41	-1.171	22.070	35.673	1.00 36.17	CPS4
ATOM	3126	CD2		41	-2.291	20.309	37.050	1.00 36.43	CPS4
ATOM	3127	C	LEU	41	-5.939	22.709	36.916	1.00 38.96	CPS4
ATOM	3128	0	LEU	41	-6.744	23.295	36.197	1.00 38.34	CPS4
ATOM	3129	N	SER	42	-5.830	22.936	38.220	1.00 39.70	CPS4
ATOM	3130	CA	SER	42	-6.645	23.937	38.890	1.00 41.21	CPS4
ATOM	3131	CB	SER	42	-6.456	23.849	40.408	1.00 41.87	CPS4
ATOM	3132	OG	SER	42	-5.119	24.152	40.781	1.00 40.52	CPS4
ATOM	3133	C	SER	42	-6.182	25.305	38.399	1.00 42.49	CPS4
ATOM	3134	0	SER	42	-5.134	25.424	37.766	1.00 42.26	CPS4



SEP 0 9 2002

FIG. 1A-55

F1G.	SUBCLASS	
0.6.	CL.538	
APPROVED	20	DRAFTSMAH

ATOM	3135	N	GLU	43	-6.955	26.338	38.703	1.00 42.87	CPS4
ATOM	3136	CA	GLU	43	-6.616	27.687	38.286	1.00 44.09	CPS4
ATOM	3137	CB	GLU	43	-7.686	28.651	38.803	1.00 46.92	CPS4
ATOM	3138	CG	GLU	43	-7.721	30.000	38.115	1.00 51.91	CPS4
ATOM	3139	CD	GLU	43	-6.722	30.982	38.687	1.00 55.38	CPS4
ATOM	3140		GLU	43	-6.747	31.203	39.920	1.00 57.45	CPS4
ATOM	3141	OE2		43	-5.920	31.543	37.905	1.00 57.72	
ATOM	3142	c	GLU	43	-5.226	28.088	38.802	1.00 43.04	CPS4
ATOM	3143	ō	GLU	43	-4.404	28.633	38.058		CPS4
ATOM	3144	N	LYS	44	-4.965	27.805	40.074	1.00 42.48	CPS4
ATOM	3145	CA	LYS	44	-3.684	28.136		1.00 41.59	CPS4
ATOM	3146	CB	LYS	44	-3.758		40.690	1.00 40.46	CPS4
ATOM	3147	CG	LYS	44		27.910	42.201	1.00 42.16	CPS4
ATOM	3148	CD	LYS		-2.528	28.378	42.960	1.00 44.29	CPS4
ATOM				44	-2.684	28.137	44.457	1.00 47.29	CPS4
ATOM	3149 3150	CE	LYS	44	-1.439	28.574	45.218	1.00 48.62	CPS4
		NZ	LYS	44	-1.554	28.319	46.683	1.00 50.30	CPS4
ATOM	3151	С	LYS	44	-2.537	27.311	40.107	1.00 38.58	CPS4
ATOM	3152	0	LYS	44	-1.466	27.845	39.806	1.00 37.53	CPS4
ATOM	3153	N	ARG	45	-2.764	26.010	39.957	1.00 35.62	CPS4
ATOM	3154	CA	ARG	45	-1.755	25.115	39.406	1.00 34.29	CPS4
MOTA	3155	CB	ARG	45	-2.205	23.663	39.575	1.00 36.05	CPS4
ATOM	3156	CG	ARG	45	-2.054	23.119	41.002	1.00 39.56	CPS4
ATOM	3157	CD	ARG	45	-0.605	22.768	41.301	1.00 42.27	CPS4
ATC::	3158	NE	ARG	4.5	-0.090	21.793	40.341	1.00 45.82	CPS4
MOTA	3159	CZ	ARG	4.5	1.003	21.973	39.600	1.00 48.25	CPS4
ATOM	3160	NH1	ARG	45	1.711	23.093	39.707	1.00 47.45	CPS4
ATOM	3161	NH2	ARG	45	1.381	21.037	38.733	1.00 48.96	CPS4
ATOM	3162	C	ARG	. 45	-1.491	25.422	37.926	1.00 32.63	CPS4
ATOM	3163	0	ARG	4.5	-0.383	25.215	37.425	1.00 30.48	CPS4
ATOM	3164	N	LYS	46	-2.513	25.912	37.232	1.00 30.94	CPS4
ATOM	3165	CA	LYS	46	-2.365	26.265	35.820	1.00 30.54	CPS4
ATOM	3166	CB	LYS	46	-3.672	26.841	35.262	1.00 31.76	
ATOM	3167	CG	LYS	46	-4.637	25.828	34.661	1.00 32.98	CPS4
ATOM	3168	CD	LYS	46	-5.770	26.574	33.959		CPS4
ATOM	3169	CE	LYS	46	-6.597			1.00 35.55	CPS4
ATOM	3170	NZ	LYS	46	-7.283	25.647	33.081	1.00 37.38	CPS4
ATOM	3171	c	LYS	46		24.614	33.895	1.00 39.63	CPS4
ATOM	3172	0	LYS	46	-1.275	27.326	35.668	1.00 30.10	CPS4
ATOM	3173	N	ASN		-0.365	27.197	34.843	1.00 28.86	CPS4
ATOM	3174	CA	ASN	47	-1.378	28.388	36.457	1.00 29.05	CPS4
ATOM	3175	CB		47	-0.393	29.445	36.357	1.00 29.35	CPS4
ATOM	3176	CG	ASN	47	-0.875	30.700	37.081	1.00 32.62	CPS4
ATOM			ASN	4.7	-1.923	31.471	36.270	1.00 36.22	CPS4
	3177		ASN	47	-1.748	31.710	35.065	1.00 37.87	CPS4
ATOM	3178		ASN	47	-3.008	31.869	36.928	1.00 38.04	CPS4
ATOM	3179	С	ASN	47	0.998	29.033	36.822	1.00 28.34	CPS4
ATOM	3180	0	ASN	47	1.987	29.533	36.291	1.00 26.63	CPS4
ATOM	3181	N	GLU	48	1.085	28.125	37.794	1.00 27.39	CPS4
ATOM	3182	CA	GLU	48	2.398	27.656	38.253	1.00 26.57	CPS4
ATOM	3183	CB	GLU	48	2.256	26.763	39.493	1.00 29.29	CPS4
ATOM	3184	CG	GLU	48	1.753	27.481	40.733	1.00 35.14	CPS4
ATOM	3185	CD	GLU	48	1.467	26.534	41.899	1.00 38.18	CPS4
ATOM	3186		GLU	48	1.054	27.029	42.970	1.00 39.62	CPS4
MOTA	3187	OE2	GLU	48	1.654	25.301	41.747	1.00 39.49	CPS4
ATOM	3188	С	GLU	48	3.023	26.848	37.114	1.00 39.49	CPS4
ATOM	3189	0	GLU	48	4.198	27.004	36.786	1.00 24.55	CPS4
ATOM	3190	N	PHE	49	2.215	25.984	36.513	1.00 23.53	CPS4
ATOM	3191	CA	PHE	49	2.215				
					2.643	25.136	35.400	1.00 22.71	CPS4



SEP 0 9 2002

FIG. 1A-56

≓IG.	SUBCLASS	
0.G. F	CLASS	
APPEOVED	7.0	DRAFTSMAN

ATOM	3192	CB	PHE	49	1.474	24.235	34.972	1.00 23.78	CPS4
ATOM	3193	CG	PHE	49	1.796	23.299	33.836	1.00 23.79	CPS
ATOM	3194	CD1	PHE	49	2.359	22.053	34.084	1.00 25.06	CPS
ATOM	3195	CD2	PHE	49	1.525	23.660	32.522	1.00 24.25	CPS
ATOM	3196		PHE	49	2.645	21.179	33.045	1.00 25.26	CPS4
ATOM	3197	CE2	PHE	49	1.812	22.786	31.464	1.00 25.16	CPS4
ATOM	3198	cz	PHE	49	2.370	21.546	31.729	1.00 26.61	CPS
ATOM	3199	c	PHE	49	3.089	25.980	34.201	1.00 22.04	CPS4
ATOM	3200	ō	PHE	49	4.158	25.751	33.631	1.00 21.19	
ATOM	3201	N	LEU	50	2.260	26.945	33.818	1.00 21.19	CPS4
ATOM	3202	CA	LEU	50	2.564	27.807	32.678		CPS4
ATOM	3203	CB	LEU	50	1.386	28.749		1.00 21.41	CPS4
ATOM	3204	CG	LEU	50	1.487	29.682	32.389	1.00 21.73	CPS4
ATOM	3205		LEU	50			31.172	1.00 24.05	CPS4
ATOM	3206		LEU		1.697	28.873	29.891	1.00 24.04	CPS4
				50	0.218	30.518	31.075	1.00 23.32	CPS4
ATOM	3207	C	LEU	50	3.832	28.624	32.922	1.00 21.21	CPS4
ATOM	3208	0	LEU	50	4.680	28.724	32.039	1.00 20.96	CPS
ATOM	3209	N	ALA	51	3.960	29.207	34.114	1.00 19.78	CPS4
ATOM	3210	CA	ALA	51	5.150	30.005	34.432	1.00 19.68	CPS4
ATOM	3211	CB	ALA	51	5.017	30.616	35.830	1.00 20.19	CPS
ATOM	3212	С	ALA	51	6.417	29.151	34.350	1.00 20.59	CPS
ATOM	3213	0	ALA	51	7.453	29.598	33.830	1.00 20.05	CPS
ATOM	3214	N	GLY	52	6.325	27.928	34.865	1.00 20.38	CPS
ATOM	3215	CA	GLY	52	7.459	27.015	34.840	1.00 20.83	CPS-
ATOM	3216	C	GLY	52	7.861	26.619	33.429	1.00 20.53	CPS
ATOM	3217	0	GLY	52	9.048	26.587	33.104	1.00 20.29	CPS
ATOM	3218	N	ARG	53	6.884	26.279	32.593	1.00 21.19	CPS
ATOM	3219	CA	ARG	53	7.187	25.916	31.207	1.00 21.65	CPS
ATOM	3220	CB	ARG	53	5.938	25.336	30.532	1.00 23.50	CPS
ATOM	3221	CG	ARG	53	5.824	23.807	30.654	1.00 26.67	CPS
ATOM	3222	CD	ARG	53	5.988	23.291	32.077	1.00 31.06	CPS4
ATOM	3223	NE	ARG	53	5.877	21.832	32.121	1.00 35.13	CPS4
ATOM	3224	CZ	ARG	53	6.220	21.082	33.164	1.00 38.06	CPS4
ATOM	3225	NH1	ARG	53	6.702	21.649	34.267	1.00 38.57	CPS4
ATOM .	3226		ARG	53	6.086	19.762	33.105	1.00 39.34	CPS4
ATOM	3227	С	ARG	53	7.710	27.140	30.445	1.00 20.71	CPS
ATOM	3228	ō	ARG	53	8.598	27.030	29.606	1.00 20.71	CPS4
ATOM	3229	N	PHE	54	7.160	28.311	30.740	1.00 20.84	CPS4
ATOM	3230	CA	PHE	54	7.613	29.545			
ATOM	3231	CB	PHE	54	6.742		30.090	1.00 19.84	CPS4
ATOM	3232	CG	PHE	54	7.131	30.722 32.059	30.558	1.00 19.76	CPS4
ATOM	3233	CD1		54			29.966	1.00 22.53	CPS4
ATOM	3234	CD2		54	7.984	32.922	30.654	1.00 21.19	CPS4
ATOM	3235	CE1		54	6.638	32.457	28.728	1.00 22.55	CPS4
ATOM	3236	CE2			8.339	34.162	30.115	1.00 22.92	CPS4
ATOM				54	6.989	33.701	28.181	1.00 24.30	CPS4
ATOM	3237	cz	PHE	54	7.846	34.553	28.883	1.00 22.82	CPS4
	3238	C	PHE	54	9.086	29.791	30.452	1.00 20.51	CPS4
ATOM	3239	0	PHE	54	9.912	30.084	29.583	1.00 19.99	CPS4
ATOM	3240	N	ALA	55	9.419	29.656	31.735	1.00 19.95	CPS4
ATOM	3241	CA	ALA	55	10.798	29.874	32.179	1.00 18.42	CPS4
ATOM	3242	CB	ALA	55	10.885	29.789	33.712	1.00 17.59	CPS4
ATOM	3243	С	ALA	55	11.747	28.867	31.535	1.00 18.74	CPS4
ATOM	3244	0	ALA	55	12.840	29.228	31.097	1.00 17.86	CPS4
ATOM	3245	N	ALA	56	11.329	27.608	31.470	1.00 17.67	CPS4
ATOM	3246	CA	ALA	5 6	12.173	26.570	30.870	1.00 17.97	CPS4
ATOM	3247	CB	ALA	56	11.519	25.179	31.051	1.00 16.50	CPS4
ATOM	3248	С	ALA	56	12.435	26.845	29.391	1.00 17.61	CPS4



SEP 0 9 2002

FIG. 1A-57

TECH CENTER 1600/2900

65	SUBCLASS	
0.6. FIG	CLASS SUR	
APPROVED	10	MART DERAN

ATOM	3249	0	ALA	56	13.555
ATOM	3250	N	LYS	57	11.411
ATOM	3251	CA	LYS	57	11.603
ATOM	3252	СВ	LYS	57	10.243
ATOM	3253	CG	LYS	57	9.470
ATOM	3254	CD	LYS	57	8.243
ATOM	3255	CE	LYS		
ATOM	3256	NZ		57	7.453
ATOM			LYS	57	6.468
	3257	C	LYS	57	12.450
ATOM	3258	0	LYS	57	13.282
ATOM	3259	N	GLU	58	12.254
ATOM	3260	CA	GLU	58	13.057
ATOM	3261	CB	GLU	58	12.581
ATOM	3262	CG	GLU	58	11.276
ATOM	3263	CD	GLU	58	11.375
ATOM	3264	OE1	GLU	58	12.482
ATOM	3265	OE2	GLU	58	10.333
ATOM	3266	С	GLU	58	14.504
ATOM	3267	0	GLU	58	15.424
ATOM	3268	N	ALA	59	14.718
ATOM	3269	CA	ALA	59	16.095
ATOM	3270	CB	ALA	59	16.130
ATOM	3271	C	ALA	59	
ATOM	3272	0	ALA		16.704
ATOM	3272			59	17.868
ATOM	3274	N	PHE	60	15.925
		CA	PHE	60	16.438
ATOM ATOM	3275	CB	PHE	60	15.404
	3276	CG	PHE	60	15.860
ATOM	3277	CD1	PHE	60	16.682
ATOM	3278	CD2	PHE	60	15.565
ATOM	3279	CE1	PHE	60	17.214
ATOM	3280	CE2	PHE	60	16.092
ATOM	3281	CZ	PHE	60	16.922
ATOM	3282	С	PHE	60	16.817
ATOM	3283	0	PHE	60	17.853
ATOM	3284	N	SER	61	15.983
ATOM	3285	CA	SER	61	16.263
ATOM	3286	CB	SER	61	15.069
ATOM	3287	OG	SER	61	15.017
ATOM	3288	С	SER	61	17.554
ATOM	3289	0	SER	61	18.257
ATOM	3290	N	LYS	62	17.873
ATOM	3291	CA	LYS	62	19.095
ATOM	3292	CB	LYS	62	19.021
ATOM	3293	CG	LYS	62	17.939
ATOM	3294	CD	LYS	62	
ATOM	3295	CE	LYS	62	17.990
ATOM	3296	NZ			17.112
ATOM	3297	C	LYS	62	17.485
ATOM			LYS	62	20.309
ATOM	3298	0	LYS	62	21.375
ATOM	3299	N	ALA	63	20.156
	3300	CA	ALA	63	21.248
ATOM	3301	CB	ALA	63	20.878
ATOM	3302	С	ALA	63	21.497
ATOM	3303	0	ALA	63	22.640
ATOM	3304	N	PHE	64	20.412
ATOM	3305	CA	PHE	64	20.480

			IECH CENT	:R 1600/
13.555	26.672	28.898	1.00 17.56	CPS4
11.411	27.286	28.669	1.00 17.23	CPS4
11.603	27.555	27.249	1.00 17.45	CPS4
10.243	27.657	26.535	1.00 17.90	CPS4
9.470	26.320	26.585	1.00 17.50	CPS4
8.243	26.286	25.673	1.00 19.16	CPS4
7.453	24.998	25.915	1.00 20.14	CPS4
6.468	24.688	24.832	1.00 18.82	CPS4
12.450	28.800	27.033	1.00 18.57	CPS4
13.282	28.840	26.123	1.00 18.35	CPS4
12.254 13.057	29.815	27.863	1.00 19.33	CPS4
12.581	31.018	27.733	1.00 19.47	CPS4
11.276	32.104	28.698	1.00 21.46	CPS4
11.375	33.576	28.308 27.003	1.00 24.96	CPS4
12.482	34.040	26.654	1.00 28.39 1.00 30.73	CPS4
10.333	33.748	26.333		CPS4
14.504	30.649	28.047	1.00 31.57 1.00 19.45	CPS4
15.424	31.075	27.338	1.00 19.45	CPS4 CPS4
14.718	29.857	29.097	1.00 17.21	CPS4
16.095	29.458	29.434	1.00 16.93	CPS4
16.130	28.630	30.730	1.00 16.23	CPS4
16.704	28.663	28.288	1.00 17.64	CPS4
17.868	28.871	27.917	1.00 18.71	CPS4
15.925	27.752	27.708	1.00 17.49	CPS4
16.438	26.973	26.590	1.00 17.61	CPS4
15.404	25.953	26.093	1.00 17.74	CPS4
15.860	25.203	24.869	1.00 19.99	CPS4
16.682	24.085	24.992	1.00 21.60	CPS4
15.565	25.681	23.594	1.00 21.01	CPS4
17.214	23.453	23.863	1.00 21.01	CPS4
16.092 16.922	25.059	22.452	1.00 20.43	CPS4
16.817	23.941	22.595 25.423	1.00 22.76	CPS4
17.853	27.701	24.792	1.00 16.99 1.00 18.28	CPS4
15.983	28.894	25.139	1.00 18.28	CPS4
16.263	29.801	24.026	1.00 17.54	CPS4 CPS4
15.069	30.757	23.788	1.00 18.97	CPS4
15.017	31.816	24.738	1.00 20.70	CPS4
17.554	30.586	24.261	1.00 18.58	CPS4
18.257	30.932	23.312	1.00 19.96	CPS4
17.873	30.856	25.520	1.00 17.38	CPS4
19.095	31.579	25.855	1.00 18.60	CPS4
19.021	32.120	27.281	1.00 19.12	CPS4
17.939	33.199	27.436	1.00 24.19	CPS4
17.990	33.882	28.791	1.00 27.64	CPS4
17.112	35.126	28.763	1.00 31.95	CPS4
17.485 20.309	36.123	29.784	1.00 34.09	CPS4
20.309	30.684 31.133	25.699	1.00 18.38	CPS4
20.156	29.418	25.259	1.00 19.22	CPS4
21.248	28.460	26.070 25.934	1.00 17.11 1.00 17.76	CPS4
20.878	27.114	26.619	1.00 17.76 1.00 16.67	CPS4
21.497	28.239	24.445	1.00 18.66	CPS4 CPS4
22.640	28.126	24.012	1.00 17.98	CPS4
20.412	28.183	23.672	1.00 18.77	CPS4

27.976 22.220 1.00 19.86

CPS4



SEP 0 9 2002

FIG. 1A-58

Γ.	SUBCLASS	
.G. F1G	STASS SUB	-
APPROVED !	A9	DRAFTSMAN

ATOM	3306	CB	PHE	64	19.068	27.758	21.659	1.00 21.49	CPS4
MOTA	3307	CG	PHE	64	19.049	27,258	20.239	1.00 23.19	CPS4
MOTA	3308		PHE	64	19.603	26.019	19.917	1.00 25.84	CPS4
ATOM	3309		PHE	64	18.498	28.038	19.223	1.00 24.38	CPS4
MOTA	3310		PHE	64	19.612	25.558	18.592	1.00 27.01	CPS4
MOTA	3311		PHE	64	18.495	27.595	17.897	1.00 25.99	CPS4
ATOM	3312	CZ	PHE	64	19.055	26.353	17.578	1.00 25.96	CPS4
ATOM	3313	C	PHE	64	21.142	29.177	21.547	1.00 21.18	CPS4
MOTA	3314	0	PHE	64	21.687	29.057	20.446	1.00 22.00	CPS4
ATOM	3315	N	GLY	65	21.075	30.330	22.214	1.00 20.65	CPS4
ATOM	3316	CA	GLY	65	21.711	31.547	21.735	1.00 21.45	CPS4
ATOM	3317	C	GLY	65	20.914	32.487	20.848	1.00 23.53	CPS4
ATOM	3318	0	GLY	65	21.453	33.483	20.370	1.00 24.12	CPS4
ATOM ATOM	3319	N	THR	66	19.635	32.195	20.640	1.00 22.34	CPS4
ATOM	3320	CA	THR	66	18.807	33.016	19.755	1.00 23.68	CPS4
ATOM	3321 3322	CB OG1	THR	66 66	18.176	32.144	18.667	1.00 25.10	CPS4
ATOM	3322	CG2		66	17.343 19.249	31.160	19.296	1.00 25.13	CPS4
ATOM	3323	C	THR	66		31.434	17.845	1.00 26.27	CPS4
ATOM	3324	0	THR	66	17.646 17.172	33.737 34.762	20.424 19.925	1.00 24.40	CPS4
ATOM	3325	N	GLY	67	17.172	33.199	21.546	1.00 23.79	CPS4
ATOM	3327	CA	GLY	67	16.018	33.766	22.193	1.00 23.11	CPS4 CPS4
ATOM	3328	c	GLY	67	14.822	33.766	21.391	1.00 22.95	CPS4
ATOM	3329	õ	GLY	67	14.997	32.581	20.369	1.00 23.38	CPS4
ATOM	3330	N	ILE	68	13.610	33.540	21.848	1.00 24.83	CPS4
ATOM	3331	CA	ILE	68	12.401	33.107	21.150	1.00 25.43	CPS4
ATOM	3332	CB	ILE	68	11.194	33.083	22.110	1.00 25.71	CPS4
ATOM	3333		ILE	68	9.899	32.729	21.345	1.00 26.85	CPS4
ATOM	3334	CG1	ILE	68	11.449	32.061	23.222	1.00 24.50	CPS4
ATOM	3335	CD1	ILE	68	11.495	30.626	22.739	1.00 24.17	CPS4
ATOM	3336	С	ILE	68	12.129	34.086	20.007	1.00 27.56	CPS4
ATOM	3337	0	ILE	68	12.150	35.300	20.203	1.00 27.28	CPS4
ATOM	3338	N	GLY	69	11.890	33.559	18.813	1.00 27.53	CPS4
ATOM	3339	CA	GLY	69	11.641	34.434	17.686	1.00 30.15	CPS4
ATOM	3340	C	GLY	69	11.685	33.725	16.353	1.00 30.54	CPS4
MOTA	3341	0	GLY	69	11.274	32.575	16.240	1.00 30.54	CPS4
MOTA	3342	N	ALA	70	12.197	34.416	15.342	1.00 32.70	CPS4
MOTA	3343	CA	ALA	70	12.272	33.860	13.998	1.00 33.34	CPS4
ATOM	3344	CB	ALA	70	12.396	34.886	13.043	1.00 35.40	CPS4
ATOM	3345	С	ALA	70	13.038	32.551	13.917	1.00 33.51	CPS4
ATOM	3346	0	ALA	70	12.695	31.679	13.118	1.00 34.32	CPS4
MOTA	3347	N	GLN	71	14.061	32.398	14.752	1.00 32.10	CPS4
MOTA	3348	CA	GLN	71	14.882	31.192	14.713	1.00 30.79	CPS4
ATOM	3349	CB	GLN	71	16.334	31.545	15.039	1.00 33.45	CPS4
ATOM	3350	CG	GLN	71	16.936	32.597	14.127	1.00 37.57	CPS4
MOTA	3351	CD	GLN	71	18.391	32.873	14.451	1.00 38.92	CPS4
ATOM ATOM	3352		GLN	71	19.258	32.016	14.257	1.00 40.93	CPS4
	3353	NE2	GLN	71	18.665	34.069	14.961	1.00 40.14	CPS4
ATOM ATOM	3354	C	GLN	71	14.443	30.066	15.636	1.00 28.73	CPS4
ATOM	3355	O N	GLN	71	14.851	28.923	15.454	1.00 28.34	CPS4
ATOM	3356 3357		LEU	72	13.626	30.384	16.633	1.00 26.49	CPS4
ATOM	3357	CA	LEU	72	13.182	29.369	17.575	1.00 24.09	CPS4
ATOM	3358	CG	LEU	72 72	14.224	29.221	18.690	1.00 24.17	CPS4
ATOM	3360		LEU	72 72	13.988	28.183	19.791	1.00 23.09	CPS4
ATOM	3361		LEU	72	14.211	26.785	19.231	1.00 23.74	CPS4
ATOM	3362	CD2	LEU	72	14.948	28.457	20.955	1.00 25.05	CPS4
-11011	3302	_	العط	12	11.847	29.777	18.169	1.00 23.32	CPS4



RECEIVED SEP 0 9 2002

TECH CENTER 1600/2900

FIG. 1A-59

APPROVED O.G. F.IG.
61 ULASS SUBCLASS
GRAFTSHAM

MOTA	3363	0	LEU	72	11.699	30.876	18.688	1.00 24.09	CPS4
ATOM	3364	N	SER	73	10.880	28.877	18.084	1.00 22.99	CPS4
ATOM	3365	CA	SER	73	9.542	29.112	18.601	1.00 23.16	CPS4
ATOM	3366	CB	SER	73	8.527	28.653	17.555	1.00 23.80	CPS4
ATOM	3367	OG	SER	73	7.227	28.611	18.093	1.00 29.93	CPS4
ATOM	3368	С	SER	73	9.297	28.339	19.896	1.00 22.31	CPS4
ATOM	3369	0	SER	73	9.976	27.353	20.175	1.00 21.09	CPS4
ATOM	3370	N	PHE	74	8.334	28.803	20.692	1.00 22.33	CPS4
ATOM	3371	CA	PHE	74	7.962	28.093	21.914	1.00 21.01	CPS4
ATOM	3372	CB	PHE	74	6.802	28.801	22.625	1.00 21.02	CPS4
ATOM	3373	CG	PHE	74	7.201	30.032	23.386	1.00 23.04	CPS4
ATOM	3374		PHE	74	8.018	29.937	24.508	1.00 23.64	CPS4
ATOM	3375		PHE	74	6.726	31.285	23.003	1.00 22.57	CPS4
ATOM	3376		PHE	74	8.355	31.074	25.246	1.00 25.06	CPS4
ATOM	3377	CE2		74	7.057	32.423	23.728	1.00 25.56	CPS4
ATOM	3378	cz	PHE	74	7.872	32.318	24.854	1.00 24.29	CPS4
ATOM	3379	c	PHE	74	7.470	26.714	21.479	1.00 21.66	CPS4
ATOM	3380	ō	PHE	74	7.567	25.744	22.224	1.00 21.66	
ATOM	3381	N	GLN	75	6.928	26.635	20.266	1.00 20.92	CPS4
ATOM	3382	CA	GLN	75	6.402	25.372			CPS4
ATOM	3383	CB	GLN	75	5.442	25.637	19.760	1.00 21.28	CPS4
ATOM	3384	CG	GLN	75	4.216	26.457	18.595 18.996	1.00 22.50	CPS4
ATOM	3385	CD	GLN	75	3.364	25.763		1.00 22.28	CPS4
ATOM	3386	OE1		75	2.914	26.384	20.048	1.00 22.84	CPS4
ATOM	3387	NE2	GLN	75	3.133	24.471	21.020 19.858	1.00 25.78	CPS4
ATOM	3388	C	GLN	75	7.482	24.471	19.334	1.00 21.79	CPS4
ATOM	3389	ō	GLN	75	7.179	23.209	19.334	1.00 21.34	CPS4
ATOM	3390	N	ASP	76	8.732	24.835	19.072	1.00 22.34	CPS4
ATOM	3391	CA	ASP	76	9.872	23.989	18.903	1.00 20.43	CPS4 CPS4
ATOM	3392	CB	ASP	76	11.006	24.827	18.294	1.00 20.89	
ATOM	3393	CG	ASP	76	10.672	25.375	16.234	1.00 25.59	CPS4
ATOM	3394	OD1	ASP	76	10.016	24.658	16.149	1.00 28.36	CPS4
ATOM	3395	OD2	ASP	76	11.094	26.513	16.614	1.00 25.63	CPS4
ATOM	3396	c	ASP	76	10.442	23.292	20.132	1.00 20.74	CPS4 CPS4
MOTA	3397	ō	ASP	76	11.380	22.499	20.132	1.00 20.74	
ATOM	3398	N	ILE	77	9.869	23.586	21.291	1.00 20.53	CPS4 CPS4
ATOM	3399	CA	ILE	77	10.353	23.033	22.551	1.00 19.49	CPS4
ATOM	3400	CB	ILE	77	10.944	24.160	23.433	1.00 18.31	
ATOM	3401	CG2		77	11.700	23.554	24.627	1.00 19.88	CPS4 CPS4
ATOM	3402	CG1	ILE	77	11.856	25.056	22.584	1.00 19.88	CPS4
ATOM	3403	CD1	ILE	77	12.172	26.401	23.232	1.00 19.12	
ATOM	3404	C	ILE	77	9.249	22.387	23.232	1.00 18.75	CPS4 CPS4
ATOM	3405	ō	ILE	77	8.162	22.932	23.474	1.00 20.14	CPS4
ATOM	3406	N	GLU	78	9.530	21.233	23.942	1.00 20.14	CPS4
ATOM	3407	CA	GLU	78	8.520	20.590	24.760	1.00 20.14	CPS4
ATOM	3408	CB	GLU	78	7.814	19.483	23.964	1.00 22.66	CPS4
ATOM	3409	CG	GLU	78	6.792	18.707	24.772	1.00 23.61	CPS4
ATOM	3410	CD	GLU	78	5.914	17.815	23.903	1.00 26.69	CPS4
ATOM	3411		GLU	78	5.039	18.352	23.195	1.00 26.76	CPS4
ATOM	3412		GLU	78	6.105	16.581	23.922	1.00 27.97	CPS4
ATOM	3413	c	GLU	78	9.153	20.025	26.014	1.00 27.97	CPS4
ATOM	3414	ō	GLU	78	10.219	19.411	25.953	1.00 20.86	CPS4
ATOM	3415	и	ILE	79	8.519	20.273	27.158	1.00 20.47	CPS4
ATOM	3416	CA	ILE	79	9.019	19.744	28.420	1.00 20.88	CPS4
ATOM	3417	CB	ILE	79	8.845	20.756	29.598	1.00 21.74	CPS4
ATOM	3418	CG2		79	9.053	20.756	30.937	1.00 23.26	CPS4
ATOM	3419		ILE	79	9.868	21.891	29.485	1.00 23.26	CPS4
	,			,,,	3.008	21.031	27.405	1.00 27.28	CP34



SEP 0 9 2002

FIG. 1A-60

.G. F1G.	DLASS SUBCLASS	1
APPROVED D	, Ng	DRAFTSHAN

MOTA	3420	CD1	ILE	79	9.772	22.726	28.227	1.00 28.49	CPS4
MOTA	3421	C	ILE	79	8.234	18.478	28.748	1.00 22.41	CPS4
ATOM	3422	0	ILE	79 .	7.001	18.462	28.685	1.00 22.59	CPS4
MOTA	3423	N	ARG	80	8.958	17.417	29.075	1.00 22.76	CPS4
ATOM	3424	CA	ARG	80	8.349	16.151	29.451	1.00 24.99	CPS4
ATOM	3425	CB	ARG	80	8.684	15.081	28.419	1.00 25.33	CPS4
MOTA	3426	CG	ARG	80	8.181	15.426	27.038	1.00 28.31	CPS4
MOTA	3427	CD	ARG	80	8.496	14.332	26.049	1.00 31.70	CPS4
MOTA	3428	NE	ARG	80	7.736	14.538	24.828	1.00 33.61	CPS4
ATOM	3429	CZ	ARG	80	7.701	13.677	23.820	1.00 35.93	CPS4
ATOM	3430		ARG	80	8.390	12.545	23.893	1.00 34.86	CPS4
MOTA	3431	NH2		80	6.974	13.952	22.743	1.00 35.80	CPS4
MOTA	3432	С	ARG	80	8.938	15.777	30.802	1.00 26.08	CPS4
ATOM	3433	0	ARG	80	9.892	16.412	31.257	1.00 22.69	CPS4
ATOM	3434	N	LYS	81	8.372	14.760	31.448	1.00 27.41	CPS4
ATOM	3435	CA	LYS	81	8.877	14.334	32.750	1.00 29.89	CPS4
ATOM	3436	CB	LYS	81	7.866	14.652	33.858	1.00 31.74	CPS4
ATOM	3437	CG	LYS	81	7.741	16.134	34.201	1.00 36.20	CPS4
ATOM	3438	CD	LYS	81	6.836	16.335	35.421	1.00 39.03	CPS4
ATOM	3439	CE	LYS	81	6.576	17.813	35.724	1.00 41.06	CPS4
ATOM	3440	NZ	LYS	81	7.812	18.590	36.021	1.00 41.14	CPS4
ATOM	3441	С	LYS	81	9.157	12.844	32.742	1.00 31.20	CPS4
ATOM	3442	0	LYS	81	8.378	12.069	32.185	1.00 30.64	CPS4
MOTA	3443	N	ASP	82	10.270	12.432	33.341	1.00 30.63	CPS4
ATOM	3444	CA	ASP	82	10.567	11.010	33.374	1.00 31.88	CPS4
ATOM	3445	CB	ASP	82	12.073	10.746	33.491	1.00 30.04	CPS4
ATOM ATOM	3446	CG	ASP	82	12.670	11.248	34.788	1.00 30.81	CPS4
ATOM	3447		ASP	82	11.938	11.421	35.789	1.00 31.13	CPS4
ATOM	3448 3449		ASP	82	13.899	11.447	34.805	1.00 31.19	CPS4
ATOM	3449	C	ASP	82	9.820	10.351	34.523	1.00 32.86	CPS4
ATOM	3451	0	ASP	82	9.037	10.997	35.221	1.00 32.72	CPS4
ATOM	3452	CA	GLN GLN	83 83	10.063 9.404	9.059 8.292	34.710 35.755	1.00 35.26	CPS4
ATOM	3453	CB	GLN	83	9.404	6.827		1.00 37.75	CPS4
ATOM	3454	CG	GLN	83	11.357	6.615	35.684 35.407	1.00 40.68	CPS4
ATOM	3455	CD	GLN	83	11.805	7.096	34.020	1.00 45.63	CPS4 CPS4
ATOM	3456	OE1	GLN	83	11.016	7.130	33.068	1.00 49.44	CPS4
ATOM	3457	NE2		83	13.086	7.447	33.901	1.00 50.02	CPS4
ATOM	3458	C	GLN	83	9.607	8.854	37.160	1.00 38.09	CPS4
ATOM	3459	ō	GLN	83	8.748	8.688	38.026	1.00 38.46	CPS4
ATOM	3460	N	ASN	84	10.733	9.528	37.386	1.00 37.38	CPS4
ATOM	3461	CA	ASN	84	11.012	10.119	38.692	1.00 36.22	CPS4
ATOM	3462	CB	ASN	84	12.520	10.213	38.931	1.00 37.16	CPS4
ATOM	3463	CG	ASN	84	13.170	8.858	39.110	1.00 37.93	CPS4
ATOM	3464	OD1	ASN	84	12.631	7.984	39.787	1.00 39.18	CPS4
MOTA	3465	ND2	ASN	84	14.343	8.682	38.518	1.00 39.57	CPS4
ATOM	3466	С	ASN	84	10.404	11.512	38.834	1.00 36.01	CPS4
ATOM	3467	0	ASN	84	10.470	12.118	39.903	1.00 37.22	CPS4
MOTA	3468	N	GLY	85	9.817	12.027	37.759	1.00 34.03	CPS4
MOTA	3469	CA	GLY	85	9.226	13.352	37.824	1.00 31.62	CPS4
MOTA	3470	C	GLY	85	10.203	14.446	37.408	1.00 29.19	CPS4
MOTA	3471	0	GLY	85	9.904	15.632	37.517	1.00 28.96	CPS4
MOTA	3472	N	LYS	86	11.377	14.048	36.938	1.00 26.53	CPS4
MOTA	3473	CA	LYS	86	12.394	15.009	36.507	1.00 25.85	CPS4
MOTA	3474	CB	LYS	86	13.775	14.336	36.511	1.00 26.12	CPS4
MOTA	3475	CG	LYS	86	14.913	15.136	35.853	1.00 24.62	CPS4
MOTA	3476	CD	LYS	86	15.358	16.357	36.678	1.00 22.52	CPS4



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-61

APROVED 0.G F1G.

BY CLASS SUBCLASS

ORAFISHAN

MOTA	3477	CE	LYS	86	16.368	17.189	35.880	1.00 23.49	CPS4
ATOM	3478	NZ	LYS	86	17.044	18.252	36.687	1.00 21.98	CPS4
ATOM	3479	С	LYS	86	12.069	15.527	35.105	1.00 25.27	CPS4
ATOM	3480	0	LYS	86	11.868	14.746	34.175	1.00 23.72	CPS4
ATOM	3481	N	PRO	87	11.987	16.859	34.936	1.00 24.18	CPS4
ATOM	3482	CD	PRO	87	12.068	17.970	35.906	1.00 24.38	CPS4
ATOM	3483	CA	PRO	87	11.682	17.351	33.589	1.00 23.07	CPS4
ATOM	3484	CB	PRO	87	11.343	18.825	33.822	1.00 24.68	CPS4
ATOM	3485	CG	PRO	87	12.229	19.189	34.995	1.00 24.14	CPS4
ATOM	3486	С	PRO	87	12.869	17.202	32.658	1.00 22.51	CPS4
ATOM	3487	0	PRO	87	14.028	17.182	33.098	1.00 21.21	CPS4
ATOM	3488	N	TYR	88	12.576	17.094	31.366	1.00 21.14	CPS4
MOTA	3489	CA	TYR	88	13.617	17.009	30.363	1.00 21.50	CPS4
MOTA	3490	CB	TYR	88	14.069	15.563	30.132	1.00 23.25	CPS4
ATOM	3491	CG	TYR	88	13.032	14.648	29.546	1.00 24.04	CPS4
MOTA	3492		TYR	88	12.953	14.449	28.165	1.00 26.52	CPS4
ATOM	3493		TYR	88	12.033	13.554	27.622	1.00 27.83	CPS4
ATOM	3494		TYR	88	12.164	13.941	30.369	1.00 25.98	CPS4
ATOM	3495	CE2	TYR	88	11.241	13.048	29.840	1.00 27.07	CPS4
ATOM	3496	cz	TYR	88	11.185	12.857	28.467	1.00 27.07	CPS4
ATOM	3497	ОН	TYR	88	10.295	11.941	27.945	1.00 20.72	CPS4
ATOM	3498	c	TYR	88	13.049	17.631	29.105	1.00 20.69	CPS4
MOTA	3499	ō	TYR	88	11.839	17.679	28.915	1.00 20.95	CPS4
ATOM	3500	N	ILE	89	13.930	18.130	28.257	1.00 20.33	CPS4
ATOM	3501	CA	ILE	89	13.501	18.805	27.042	1.00 21.21	CPS4
ATOM	3502	CB	ILE	89	14.275	20.141	26.878	1.00 20.12	CPS4
ATOM	3503		ILE	89	14.157	20.667	25.423	1.00 20.12	CPS4
ATOM	3504	CG1		89	13.757	21.164	27.900	1.00 20.90	CPS4
ATOM	3505		ILE	89	14.595	22.440	28.000	1.00 20.90	CPS4
ATOM	3506	c	ILE	89	13.698	18.011.	25.767	1.00 21.80	CPS4
ATOM	3507	ō	ILE	89	14.685	17.290	25.625	1.00 22.10	CPS4
ATOM	3508	N	ILE	90	12.729	18.126	24.862	1.00 22.64	CPS4
ATOM	3509	CA	ILE	90	12.871	17.544	23.538	1.00 23.23	CPS4
ATOM	3510	CB	ILE	90	11.850	16.413	23.228	1.00 25.32	CPS4
ATOM	3511		ILE	90	11.987	15.303	24.259	1.00 25.34	CPS4
MOTA	3512			90	10.424	16.946	23.187	1.00 27.66	CPS4
ATOM	3513	CD1	ILE	90	9.462	16.003	22.454	1.00 29.92	CPS4
ATOM	3514	С	ILE	90	12.609	18.760	22.654	1.00 23.52	CPS4
ATOM	3515	0	ILE	90	11.780	19.610	22.988	1.00 23.18	CPS4
ATOM	3516	N	CYS	91	13.341	18.892	21.558	1.00 22.32	CPS4
ATOM	3517	CA	CYS	91	13.118	20.042	20.692	1.00 24.32	CPS4
ATOM	3518	СВ	CYS	91	14.023	21.209	21.096	1.00 22.65	CPS4
ATOM	3519	SG	CYS	91	15.776	20.862	20.976	1.00 28.76	CPS4
ATOM	3520	С	CYS	91	13.367	19.670	19.244	1.00 24.59	CPS4
ATOM	3521	0	CYS	91	13.834	18.575	18.947	1.00 26.28	CPS4
ATOM	3522	N	THR	92	13.064	20.591	18.344	1.00 25.08	CPS4
MOTA	3523	CA	THR	92	13.234	20.325	16.920	1.00 25.00	CPS4
ATOM	3524	CB	THR	92	12.266	21.187	16.102	1.00 26.21	CPS4
MOTA	3525		THR	92	12.577	22.562	16.329	1.00 25.10	CPS4
ATOM	3526		THR	92	10.828	20.933	16.526	1.00 25.78	CPS4
ATOM	3527	c	THR	92	14.633	20.629	16.417	1.00 25.78	CPS4
ATOM	3528	ō	THR	92	14.938	20.371	15.255	1.00 26.72	CPS4
ATOM	3529	N	LYS	93	15.480	21.163	17.291	1.00 27.72	CPS4 CPS4
ATOM	3530	CA	LYS	93	16.830	21.589	16.927	1.00 28.49	CPS4
ATOM	3531	СВ	LYS	93	17.109	22.946	17.583	1.00 28.49	CPS4
ATOM	3532	CG	LYS	93	16.792	24.162	16.729	1.00 30.97	CPS4 CPS4
MOTA	3533	CD	LYS	93	15.450	24.102	16.729	1.00 38.80	CPS4
				-55	13.450	24.100	10.039	1.00 38.80	CPS4



SEP 0 9 2002

FIG. 1A-62

FIG.	SUBCLASS	
0.0	CLASS	
APFROVES	ΒX	DRAFTSMAN

ATOM	3534	CE	LYS	93	15.212	25.376	15.229	1.00 40.84	CPS4
ATOM	3535	NZ	LYS	93	14.048	25.250	14.312	1.00 43.58	CPS
ATOM	3536	С	LYS	93	18.005	20.676	17.234	1.00 27.51	CPS4
ATOM	3537	0	LYS	93	19.005	20.676	16.509	1.00 27.46	CPS4
ATOM	3538	N	LEU	94	17.910	19.911	18.307	1.00 26.01	CPS4
ATOM	3539	CA	LEU	94	19.020	19.058	18.676	1.00 25.30	CPS4
ATOM	3540	CB	LEU	94	20.055	19.904	19.408	1.00 27.33	
ATOM	3541	CG	LEU	94	19.418	20.843	20.433		CPS4
ATOM	3542		LEU	94				1.00 28.62	CPS4
ATOM	3542		LEU		19.228	20.074	21.712	1.00 30.37	CPS4
ATOM				94	20.292	22.060	20.673	1.00 30.20	CPS4
	3544	C	LEU	94	18.556	17.889	19.524	1.00 25.14	CPS4
ATOM	3545	0	LEU	94	17.414	17.854	19.974	1.00 24.61	CPS4
ATOM	3546	N	SER	95	19.460	16.944	19.755	1.00 24.28	CPS4
ATOM	3547	CA	SER	95	19.153	15.731	20.499	1.00 26.04	CPS4
ATOM	3548	CB	SER	95	20.323	14.756	20.355	1.00 27.48	CPS4
ATOM	3549	OG	SER	95	20.100	13.586	21.116	1.00 33.27	CPS
ATOM	3550	С	SER	95	18.825	15.908	21.982	1.00 25.21	CPS4
ATOM	3551	0	SER	95	19.445	16.714	22.672	1.00 26.64	CPS
ATOM	3552	N	PRO	96	17.840	15.150	22.485	1.00 25.96	CPS4
ATOM	3553	CD	PRO	96	16.943	14.229	21.760	1.00 25.56	CPS4
ATOM	3554	CA	PRO	96	17.461	15.245	23.900	1.00 26.26	CPS4
ATOM	3555	CB	PRO	96	16.385	14.165	24.045	1.00 26.57	CPS4
ATOM	3556	CG	PRO	96	15.745	14.149	22.679	1.00 27.21	
ATOM	3557	c	PRO	96	18.677	14.961	24.787		CPS4
ATOM	3558	ŏ	PRO	96	18.835	15.561		1.00 26.31	CPS4
ATOM	3559	N	ALA	97			25.856	1.00 24.59	CPS4
ATOM	3560	CA	ALA	97	19.541	14.056	24.323	1.00 27.53	CPS4
ATOM					20.739	13.678	25.074	1.00 29.07	CPS4
	3561	CB	ALA	97	21.480	12.589	24.286	1.00 34.39	CPS4
ATOM	3562	C	ALA	97	21.690	14.853	25.314	1.00 27.61	CPS4
ATOM	3563	0	ALA	97	22.492	14.827	26.251	1.00 26.14	CPS4
ATOM	3564	N	ALA	98	21.599	15.885	24.483	1.00 24.18	CPS4
ATOM	3565	CA	ALA	98	22.486	17.034	24.617	1.00 23.38	CPS4
ATOM	3566	CB	ALA	98	22.804	17.600	23.238	1.00 25.54	CPS4
ATOM	3567	С	ALA	98	21.943	18.150	25.500	1.00 23.06	CPS4
ATOM	3568	0	ALA	98	22.634	19.140	25.730	1.00 23.28	CPS4
ATOM	3569	N	VAL	99	20.720	17.993	25.999	1.00 21.46	CPS4
ATOM	3570	CA	VAL	99	20.109	19.048	26.796	1.00 20.54	CPS4
ATOM	3571	CB	VAL	99	18.806	19.548	26.146	1.00 21.70	CPS4
ATOM	3572	CG1	VAL	99	18.317	20.837	26.820	1.00 20.11	CPS4
ATOM	3573	CG2	VAL	99	19.026	19.777	24.692	1.00 25.15	CPS4
ATOM	3574	C	VAL	99	19.781	18.622	28.206	1.00 20.45	CPS4
ATOM	3575	0	VAL	99	19.399	17.477	28.450	1.00 20.26	CPS4
ATOM	3576	N	HIS	100	19.924	19.572	29.123		
ATOM	3577	CA	HIS	100	19.634			1.00 19.96	CPS4
ATOM	3578	CB	HIS	100	20.935	19.349	30.531	1.00 19.64	CPS4
ATOM	3579	CG	HIS	100		19.210	31.318	1.00 20.91	CPS4
ATOM	3580		HIS	100	21.844	18.154	30.773	1.00 24.67	CPS4
ATOM	3581				22.842	18.227	29.862	1.00 26.77	CPS4
		ND1		100	21.715	16.820	31.096	1.00 26.53	CPS4
ATOM ATOM	3582		HIS	100	22.593	16.115	30.403	1.00 26.82	CPS4
	3583	NE2		100	23.288	16.946	29.646	1.00 28.13	CPS4
ATOM	3584	С	HIS	100	18.864	20.561	31.020	1.00 18.58	CPS4
ATOM	3585	0	HIS	100	19.141	21.683	30.602	1.00 18.37	CPS4
ATOM	3586	N	VAL	101	17.907	20.336	31.911	1.00 18.87	CPS4
ATOM	358 7	CA	VAL	101	17.103	21.434	32.431	1.00 17.84	CPS4
ATOM	3588	CB	VAL	101	15.800	21.590	31.608	1.00 16.78	CPS4
ATOM	358 9	CG1	VAL	101	14.930	20.345	31.770	1.00 18.44	CPS4
ATOM	3590	CG2	VAL	101	15.029	22.840	32.049	1.00 18.77	CPS4
						_2.0.0	-2.043	2.00 10.77	CFS4



SEP 0 9 2002

FIG. 1A-63

TECH CENTER 1600/2900

APPROVED O.G. FIG.
BY CLASS SUBCLASS
DRAFTSMAN

ATOM	3591	С	VAL	101	16.723	21.199	33.879	1.00 18.74	CPS4
ATOM	3592	0	VAL	101	16.711	20.069	34.350	1.00 17.29	CPS4
ATOM	3593	N	SER	102	16.441	22.287	34.590	1.00 18.62	CPS4
ATOM	3594	CA	SER	102	15.980	22.193	35.963	1.00 18.53	CPS4
ATOM	3595	CB	SER	102	17.117	22.333	36.970	1.00 19.00	CPS4
ATOM	3596	OG	SER	102	16.596	22.169	38.289	1.00 19.73	CPS4
ATOM	3597	С	SER	102	15.004	23.348	36.139	1.00 19.67	CPS4
ATOM	3598	0	SER	102	15.250	24.446	35.638	1.00 18.04	CPS4
ATOM	3599	N	ILE	103	13.901	23.092	36.841	1.00 19.50	CPS4
ATOM	3600	CA	ILE	103	12.886	24.105	37.082	1.00 19.92	CPS4
ATOM	3601	CB	ILE	103	11.552	23.731	36.386	1.00 22.07	CPS4
ATOM	3602	CG2	ILE	103	10.527	24.867	36.551	1.00 23.01	CPS4
ATOM	3603	CG1	ILE	103	11.804	23.454	34.905	1.00 21.39	CPS4
ATOM	3604	CD1	ILE	103	10.570	22.958	34.144	1.00 21.32	CPS4
ATOM	3605	C	ILE	103	12.642	24.173	38.590	1.00 20.11	CPS4
ATOM	3606	0	ILE	103	12.633	23.137	39.277	1.00 20.14	CPS4
ATOM	3607	N	THR	104	12.462	25.386	39.098	1.00 18.69	CPS4
ATOM	3608	CA	THR	104	12.205	25.588	40.517	1.00 21.54	CPS4
ATOM	3609	CB	THR	104	13.492	26.019	41.274	1.00 23.15	CPS4
ATOM	3610	OG1	THR	104	13.245	26.008	42.686	1.00 23.24	CPS4
ATOM	3611	CG2	THR	104	13.927	27.418	40.856	1.00 22.71	CPS4
ATOM	3612	C	THR	104	11.113	26.639	40.698	1.00 21.91	CPS4
ATOM	3613	0	THR	104	10.790	27.376	39.772	1.00 19.56	CPS4
ATOM	3614	N	HIS	105	10.542	26.701	41.899	1.00 22.60	CPS4
ATOM	3615	CA	HIS	105	9.465	27.639	42.189	1.00 24.01	CPS4
ATOM	3616	CB	HIS	105	8.110	26.927	42.112	1.00 26.53	CPS4
ATOM	3617	CG	HIS	105	7.721	26.457	40.746	1.00 30.77	CPS4
ATOM	3618	CD2	HIS	105	7.892	25.262	40.130	1.00 32.51	CPS4
ATOM	3619	ND1	HIS	105	6.995	27.237	39.871	1.00 32.62	CPS4
ATOM	3620	CE1	HIS	105	6.731	26.543	38.778	1.00 32.63	CPS4
ATOM	3621	NE2	HIS	105	7.264	25.341	38.909	1.00 33.46	CPS4
ATOM	3622	C	HIS	105	9.558	28.179	43.613	1.00 24.17	CPS4
MOTA	3623	0	HIS	105	10.135	27.537	44.491	1.00 22.69	CPS4
ATOM	3624	N	THR	106	8.992	29.366	43.816	1.00 24.57	CPS4
ATOM	3625	CA	THR	106	8.856	29.967	45.147	1.00 24.52	CPS4
ATOM	3626	CB	THR	106	9.756	31.195	45.408	1.00 24.79	CPS4
ATOM	3627	OG1	THR	106	9.327	32.299	44.602	1.00 23.92	CPS4
MOTA	3628	CG2	THR	106	11.210	30.858	45.127	1.00 24.13	CPS4
ATOM	3629	С	THR	106	7.415	30.444	45.065	1.00 26.14	CPS4
ATOM	3630	0	THR	106	6.756	30.249	44.034	1.00 26.11	CPS4
MOTA	3631	N	LYS	107	6.917	31.072	46.123	1.00 26.83	CPS4
ATOM	3632	CA	LYS	107	5.539	31.546	46.115	1.00 27.90	CPS4
ATOM	3633	CB	LYS	107	5.200	32.186	47.464	1.00 30.86	CPS4
MOTA	3634	CG	LYS	107	3.756	32.658	47.573	1.00 34.83	CPS4
ATOM	3635	CD	LYS	107	3.490	33.278	48.940	1.00 39.94	CPS4
ATOM	3636	CE	LYS	107	2.024	33.649	49.117	1.00 42.44	CPS4
ATOM	3637	NZ	LYS	107	1.755	34.215	50.479	1.00 45.42	CPS4
ATOM	3638	C	LYS	107	5.250	32.541	44.994	1.00 26.50	CPS4
ATOM	3639	0	LYS	107	4.169	32.511	44.402	1.00 27.10	CPS4
ATOM	3640	N	GLU	108	6.222	33.396	44.684	1.00 24.12	CPS4
ATOM	3641	CA	GLU	108	6.050	34.436	43.672	1.00 23.55	CPS4
ATOM	3642	CB	GLU	108	6.476	35.783	44.256	1.00 27.75	CPS4
ATOM	3643	CG	GLU	108	5.755	36.152	45.530	1.00 34.21	CPS4
ATOM	3644	CD	GLU	108	4.301	36.440	45.297	1.00 39.02	CPS4
ATOM	3645	OE1		108	3.639	35.645	44.593	1.00 43.65	CPS4
ATOM	3646	OE2		108	3.813	37.463	45.823	1.00 44.70	CPS4
ATOM	3647	c	GLU	108	6.794	34.267	42.352	1.00 23.22	CPS4
		-	-20	0	0.754	52.207		2.00 20.22	CF 34



SEP 0 9 2002

FIG. 1A-64

FIG.	SS SUBCLASS	
APPROVED O.G	BY CLASS	DRAFTSMAH

ATOM	3648	0	GLU	108	6.553	35.023	41.400	1.00 22.15	CPS4
ATOM	3649	N	TYR	109	7.711	33.308	42.293	1.00 21.80	CPS4
ATOM	3650	CA	TYR	109	8.509	33.129	41.077	1.00 22.23	CPS4
ATOM	3651	CB	TYR	109	9.940	33.626	41.317	1.00 22.18	CPS4
ATOM	3652	CG	TYR	109	10.035	35.082	41.674	1.00 22.99	CPS4
ATOM	3653	CD1	TYR	109	9.984	36.062	40.688	1.00 22.71	CPS4
ATOM	3654	CE1	TYR	109	10.017	37.418	41.018	1.00 25.19	CPS4
ATOM	3655		TYR	109	10.127	35.485	43.008	1.00 25.01	CPS4
ATOM	3656	CE2	TYR	109	10.158	36.833	43.350	1.00 26.56	CPS4
ATOM	3657	CZ	TYR	109	10.101	37,793	42.349	1.00 26.58	CPS4
ATOM	3658	ОН	TYR	109	10.114	39.128	42.677	1.00 29.10	CPS4
ATOM	3659	С	TYR	109	8.625	31.713	40.569	1.00 20.65	CPS4
ATOM	3660	0	TYR	109	8.402	30.757	41.297	1.00 20.79	CPS4
ATOM	3661	N	ALA	110	8.989	31.609	39.294	1.00 21.05	CPS4
ATOM	3662	CA	ALA	110	9.280	30.334	38.654	1.00 19.88	CPS4
ATOM	3663	CB	ALA	110	8.267	29.999	37.567	1.00 21.21	CPS4
ATOM	3664	C	ALA	110	10.638	30.617	38.028	1.00 19.33	CPS4
ATOM	3665	ō	ALA	110	10.887	31.730	37.568	1.00 20.58	CPS4
ATOM	3666	N	ALA	111	11.525	29.626	38.008	1.00 18.54	CPS4
ATOM	3667	CA	ALA	111	12.842	29.834	37.423	1.00 17.54	CPS4
ATOM	3668	CB	ALA	111	13.840	30.291	38.498	1.00 17.07	CPS4
ATOM	3669	C	ALA	111	13.314	28.540	36.786	1.00 17.07	CPS4
ATOM	3670	ō	ALA	111	12.873	27.454	37.160	1.00 17.51	CPS4
ATOM	3671	N	ALA	112	14.218	28.654	35.826	1.00 17.31	CPS4
ATOM	3672	CA	ALA	112	14.721	27.471	35.161	1.00 17.15	CPS4
ATOM	3673	CB	ALA	112	13.771	27.054	34.046	1.00 16.31	CPS4
ATOM	3674	C	ALA	112	16.092	27.742	34.583	1.00 17.29	CPS4
ATOM	3675	ō	ALA	112	16.476	28.887	34.363	1.00 15.61	
ATOM	3676	N	GLN	113	16.842	26.677	34.356		CPS4
ATOM	3677	CA	GLN	113	18.148	26.829		1.00 17.66	CPS4
ATOM	3678	CB	GLN	113	19.257	26.820	33.754 34.811	1.00 17.26 1.00 19.62	CPS4
ATOM	3679	CG	GLN	113	19.419	25.510			CPS4
ATOM	3680	CD	GLN	113	20.569	25.522	35.538 36.537	1.00 23.20	CPS4
ATOM	3681	OE1		113	20.942	24.480	37.077	1.00 26.68	CPS4
ATOM	3682	NE2	GLN	113	21.121	26.697	36.798	1.00 29.56	CPS4
ATOM	3683	C	GLN	113	18.314	25.678		1.00 29.78	CPS4
ATOM	3684	0	GLN	113	17.741	24.609	32.789	1.00 17.26	CPS4
ATOM	3685	N	VAL	114	19.093		32.975	1.00 16.60	CPS4
ATOM	3686	CA	VAL	114	19.329	25.910	31.746	1.00 16.61	CPS4
ATOM	3687	CB	VAL	114	18.523	24.880	30.744	1.00 17.56	CPS4
ATOM	3688	CG1		114		25.161	29.436	1.00 17.29	CPS4
ATOM	3689	CG2	VAL	114	19.016 17.058	24.268	28.275	1.00 18.95	CPS4
ATOM	3690	C	VAL	114	20.795	24.895	29.671	1.00 19.12	CPS4
ATOM	3691	0	VAL	114	21.454	24.886	30.386	1.00 17.66	CPS4
ATOM	3692	N	VAL			25.938	30.404	1.00 17.69	CPS4
ATOM	3693	CA	VAL	115	21.309	23.696	30.104	1.00 18.00	CPS4
ATOM	3694	CB	VAL	115	22.673	23.566	29.629	1.00 18.27	CPS4
ATOM	3695	CG1		115	23.611	22.872	30.635	1.00 19.25	CPS4
ATOM	3696	CG2	VAL	115	24.962	22.560	29.939	1.00 19.98	CPS4
ATOM				115	23.845	23.762	31.841	1.00 17.55	CPS4
ATOM	3697 3698	C	VAL	115	22.597	22.696	28.378	1.00 19.07	CPS4
ATOM		N	VAL	115	21.987	21.626	28.394	1.00 20.13	CPS4
ATOM	3699 3700		ILE	116	23.197	23.170	27.293	1.00 18.54	CPS4
ATOM		CA	ILE	116	23.236	22.407	26.053	1.00 21.10	CPS4
ATOM	3701	CB	ILE	116	22.762	23.239	24.850	1.00 21.01	CPS4
ATOM	3702	CG2	ILE	116	22.921	22.420	23.563	1.00 20.56	CPS4
	3703	CG1	ILE	116	21.298	23.652	25.046	1.00 19.07	CPS4
ATOM	3704	CD1	TPE	116	20.775	24.599	23.943	1.00 18.68	CPS4



ATOM

ATOM

3760

3761

CG1 TLE

CD1 ILE

5

5

20.521

20.582

21.321

34.835

22.454 33.780 1.00 18.31

1.00 19.13

CPS 5

CPS 5

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FIG. 1A-65

ATOM 3705 C ILE 116 24.692 22.029 25.851 1.00 22.03 CPS4 ATOM 3706 0 ILE 116 25.570 22.884 25.856 1.00 21.24 CPS4 ATOM 3707 N GLU 117 24.951 20.736 25.702 1.00 25.15 CPS4 ATOM 3708 CA GLU 117 26.317 20.266 25.509 1.00 28.51 CPS4 ATOM 3709 CB GLU 117 26.469 18.835 26.012 1.00 28.70 CPS4 ATOM 3710 CG GLU 117 26.237 18.661 27.490 1.00 33.10 CPS4 ATOM 3711 CD GLU 117 26.513 17.240 27.929 1.00 34.43 CPS4 ATOM 3712 OE1 GLU 117 27.702 16.908 28.114 1.00 36.09 CPS4 ATOM 3713 OE2 GLU 117 25.545 16.458 28.070 1.00 35.59 CPS4 ATOM 3714 С GLU 117 26.677 20,279 24.041 1.00 30.50 CPS4 ATOM 3715 0 GLU 117 25.815 20.420 23.186 1.00 29.91 CPS4 ATOM 3716 N ARG 118 27.960 20.137 23.747 1.00 34.16 CPS4 ATOM 3717 CA ARG 118 28.371 20.085 22.355 1.00 38.48 CPS4 ATOM 3718 CB ARG 118 29.800 20.597 22.182 1.00 41.53 CPS4 ATOM 3719 CG ARG 118 29.971 22,069 22.549 1.00 45.64 CPS4 ATOM 3720 CD ARG 118 30.881 22.808 21.567 1.00 47.97 CPS4 ATOM 3721 NE ARG 118 30.154 23.472 20.477 1.00 50.66 CPS4 ATOM CZ 3722 ARG 118 29.372 22.860 19.585 1.00 50.73 CPS4 ATOM 3723 NH1 ARG 118 29.188 21.550 19.633 1.00 52.65 CPS4 ATOM 3724 NH2 ARG 118 28.786 23.560 18.622 1.00 51.12 CPS4 ATOM 3725 C ARG 118 28.285 18.615 21.984 1.00 40.15 CPS4 ATOM 3726 OT1 ARG 118 27.421 18.274 21.156 1.00 41.62 CPS4 ATOM 3727 OT2 ARG 118 29.063 17.816 22.555 1.00 41.20 CPS4 ATOM 3728 C GLY 1 28.742 14.952 31.117 1.00 33.66 CPS5 ATOM 3729 0 GLY 1 29.119 14.581 32.234 1.00 34.07 CPS 5 ATOM 3730 N GLY 1 30.561 13.536 30.129 1.00 37.12 CPS5 ATOM 3731 CA GLY 1 29.506 14.565 29.858 1.00 34.50 CPS 5 ATOM 3732 N ILE 2 27.654 15.692 30.948 1.00 31.08 CPS5 ATOM 3733 CA ILE 2 26.856 16.110 32.095 1.00 28.11 CPS 5 ATOM 3734 CB ILE 2 26.178 17.462 31.826 1.00 27.63 CPS5 ATOM 3735 CG2 ILE 2 25.128 17.747 32.899 1.00 24.45 CPS5 ATOM 3736 CG1 ILE 2 27.244 18.559 31.785 1.00 28.90 CPS 5 ATOM 3737 CD1 ILE 2 26.695 19.935 31.484 1.00 31.41 CPS5 ATOM 3738 С ILE 2 25.797 15.083 32.441 1.00 27.43 CPS5 ATOM 3739 0 ILE 2 25.067 14.611 31.567 1.00 27.84 CPS 5 ATOM 3740 N TYR 3 25.719 14.735 33.723 1.00 27.08 CPS5 ATOM 3741 מי TYR 3 24.737 13.768 34.198 1.00 27.10 CPS 5 ATOM 3742 CB TYR 3 25.220 13.087 35.476 1.00 30.18 CPSS ATOM 3743 CG TYR 3 24.212 12.108 36.033 1.00 34.88 CPS5 ATOM 3744 CD1 TYR 3 24.012 10.862 35.428 1.00 36.41 CPSS ATOM 3745 CE1 TYR 3 23.063 9.963 35.920 1.00 38.43 CPS 5 ATOM 3746 CD2 TYR 3 23.435 12,433 37.146 1.00 36.11 CPS 5 ATOM 3747 CE2 TYR 3 22.484 11.542 37.646 1.00 38.38 CPS 5 MOTA 3748 CZ TYR 3 22.305 10.309 37.029 1.00 39.52 CPS 5 ATOM 3749 OH TYR 3 21.378 9.418 37.530 1.00 42.62 CPS 5 ATOM 3750 C TYR 3 23.418 14.475 34.485 1.00 26.49 CPS 5 ATOM 3751 0 TYR 3 22.340 13.985 34.130 1.00 24.87 CPS5 ATOM 3752 N GI.Y 4 23.499 15.624 35.153 1.00 24.12 CPS5 ATOM 3753 CA GLY 4 22,284 16.355 35.449 1.00 22.31 CPS 5 ATOM 3754 С GLY 4 22.562 17.715 36.047 1.00 20.04 CPS 5 ATOM 3755 0 GLY 4 23.667 17.966 36.509 1.00 20.64 CPS5 ATOM 3756 N ILE 5 21.572 18.602 36.011 1.00 19.86 CPS 5 ATOM 3757 CA TLE 5 21.730 19.932 36.592 1.00 18.90 CPS5 ATOM 3758 CB ILE 5 21.865 21.055 35.523 1.00 18.93 CPS 5 ATOM 3759 CG2 ILE 5 22.936 20.676 34.510 1.00 18.22 CPS5

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SEP 0 9 2002

FIG. 1A-66

F1G.	SUBCLASS	
ei O	CLASS	
AFFEOVED	2.6	DRAFTSMAR

ATOM	3762	C	ILE	5	20.532	20.234	37.471	1.00 18.47	CPS5
ATOM	3763	0	ILE	5	19.456	19.655	37.309	1.00 17.95	CPS5
MOTA	3764	N	GLY	6	20.727	21.149	38.410	1.00 18.51	CPS5
ATOM	3765	CA	GLY	6	19.654	21.489	39.318	1.00 18.44	CPS5
MOTA	3766	C	GLY	6	19.741	22.925	39.766	1.00 18.43	CPS5
ATOM	3767	0	GLY	6	20.829	23.461	39.972	1.00 18.58	CPS5
ATOM	3768	N	LEU	7	18.572	23.530	39.916	1.00 17.51	CPS5
ATOM	3769	CA	LEU	7	18.429	24.910	40.337	1.00 18.75	CPS5
MOTA	3770	CB	LEU	7	17.977	25.769	39.146	1.00 20.12	CPS5
ATOM	3771	CG	LEU	7	17.715	27.246	39.457	1.00 20.05	CPS5
ATOM	3772	CD:	1 LEU	7	19.056	27.945	39.706	1.00 18.90	CPS5
ATOM	3773	CD	LEU	7	16.967	27.907	38.298	1.00 19.78	CPS5
ATOM	3774	С	LEU	7	17.366	24.991	41.428	1.00 19.75	CPS5
ATOM	3775	0	LEU	7	16.329	24.330	41.353	1.00 18.94	CPS5
ATOM	3776	N	ASP	8	17.626	25.797	42.450	1.00 18.42	CPS5
ATOM	3777	CA	ASP	8	16.644	25.985	43.491	1.00 20.59	CPS5
MOTA	3778	CB	ASP	8	16.823	24.969	44.625	1.00 20.53	CPS5
ATOM	3779	CG	ASP	8	15.838	25.199	45.764	1.00 25.07	CPS5
ATOM	3780	ODI	LASP	. 8	16.142	26.008	46.666	1.00 26.32	
ATOM	3781	OD2		8	14.749	24.597	45.742	1.00 26.32	CPS5
ATOM	3782	С	ASP	8	16.700	27.391	44.066	1.00 26.95	CPS5
ATOM	3783	ō	ASP	8	17.768	27.957	44.243	1.00 19.95	CPS5
ATOM	3784	N	ILE	9	15.533	27.966			CPS5
ATOM	3785	CA	ILE	9	15.456	29.275	44.309	1.00 19.58	CPS5
ATOM	3786	СВ	ILE	9	14.814		44.949	1.00 19.88	CPS5
ATOM	3787		: ILE	9	14.757	30.352	44.055	1.00 19.43	CPS5
ATOM	3788		ILE	9		31.674	44.820	1.00 19.92	CPS5
ATOM	3789		ILE	9	15.640	30.524	42.776	1.00 18.89	CPS5
ATOM	3790	C	ILE	9	15.018	31.488	41.770	1.00 19.11	CPS5
ATOM	3791	0	ILE	9	14.538	29.012	46.121	1.00 20.96	CPS5
ATOM	3792	N	THR		13.482	28.392	45.964	1.00 20.32	CPS5
ATOM	3793	CA		10	14.950	29.453	47.301	1.00 20.95	CPS5
ATOM	3794	CB	THR	10	14.145	29.250	48.491	1.00 22.53	CPS5
ATOM	3795		THR	10	14.837	28.265	49.452	1.00 23.91	CPS5
ATOM	3796		THR	10	14.913	26.976	48.821	1.00 24.32	CPS5
ATOM				10	14.045	28.138	50.764	1.00 24.45	CPS5
ATOM	3797	C	THR	10	13.893	30.567	49.207	1.00 23.06	CPS5
ATOM	3798	0	THR	10	14.810	31.375	49.398	1.00 22.57	CPS5
ATOM	3799	N	GLU	11	12.641	30.782	49.588	1.00 23.52	CPS5
ATOM	3800	CA	GLU	11	12.260	31.997	50.302	1.00 24.89	CPS5
ATOM	3801	CB	GLU	11	10.747	32.212	50.168	1.00 25.23	CPS5
	3802	CG	GLU	11	10.217	33.456	50.870	1.00 27.69	CPS5
ATOM	3803	CD	GLU	11	8.701	33.491	50.901	1.00 29.32	CPS5
ATOM	3804		GLU	11	8.079	32.418	50.756	1.00 30.90	CPS5
ATOM	3805		GLU	11	8.129	34.584	51.089	1.00 33.76	CPS5
ATOM	3806	С	GLU	11	12.668	31.858	51.781	1.00 24.72	CPS5
MOTA	3807	0	GLU	11	12.246	30.925	52.469	1.00 25.10	CPS5
MOTA	3808	N	LEU	12	13.510	32.772	52.252	1.00 24.85	CPS5
ATOM	3809	CA	LEU	12	13.988	32.756	53.633	1.00 24.83	CPS5
ATOM	3810	CB	LEU	12	14.850	33.997	53.895	1.00 25.59	CPS5
ATOM	3811	CG	LEU	12	16.371	33.834	53.933	1.00 28.80	CPS5
ATOM	3812		LEU	12	16.851	32.954	52.799	1.00 28.80	CPS5
ATOM	3813		LEU	12	17.018	35.199	53.858	1.00 30.41	CPS5
ATOM	3814	С	LEU	12	12.856	32.691	54.661	1.00 26.18	CPS5
ATOM	3815	0	LEU	12	12.947	31.983	55.658	1.00 25.34	CPS5
MOTA	3816	N	LYS	13	11.788	33.432	54.403	1.00 27.19	CPS5
ATOM	3817	CA	LYS	13	10.644	33.479	55.304	1.00 29.15	CPS5
ATOM	3818	CB	LYS	13	9.634	34.508	54.777	1.00 31.29	CPS5
					1		51.77	1.00 31.23	CPSS



SEP 0 9 2002

FIG. 1A-67

ci	SUBCLASS	
0.G. FIG.	CLASS SI	-
APPROVED	>- 63	DRAFTSMAH

ATOM	3819	CG	LYS	13	8.429	34.734	55.668	1.00 36.36	CPS5
ATOM	3820	CD	LYS	13	7.596	35.907	55.154	1.00 40.04	CPS5
ATOM	3821	CE	LYS	13	6.387	36.178	56.041	1.00 42.34	CPS5
ATOM	3822	NZ	LYS	13	5.660	37.416	55.611	1.00 44.27	CPS5
ATOM	3823	С	LYS	13	9.989	32.108	55.449	1.00 29.23	CPS5
ATOM	3824	0	LYS	13	9.513	31.742	56.525	1.00 27.84	CPS5
ATOM	3825	N	ARG	14	9.971	31.345	54.362	1.00 28.90	CPS5
ATOM	3826	CA	ARG	14	9.371	30.019	54.384	1.00 29.32	CPS 5
ATOM	3827	CB	ARG	14	9.264	29.486	52.958	1.00 30.67	CPS 5
MOTA	3828	CG	ARG	14	8.489	28.186	52.828	1.00 33.67	CPS5
MOTA	3829	CD	ARG	14	8.693	27.591	51.442	1.00 36.77	CPS5
MOTA	3830	NE	ARG	14	8.435	26.157	51.442	1.00 40.83	CPS5
MOTA	3831	CZ	ARG	14	9.204	25.259	50.836	1.00 42.06	CPS5
ATOM	3832	NHl	ARG	14	10.289	25.640	50.176	1.00 40.50	CPS5
ATOM	3833	NH2	ARG	14	8.882	23.973	50.891	1.00 43.70	CPS5
ATOM	3834	C	ARG	14	10.210	29.072	55.257	1.00 28.72	CPS5
ATOM	3835	. 0	ARG	14	9.665	28.242	55.994	1.00 28.02	CPS5
ATOM	3836	N	ILE	15	11.533	29.199	55.170	1.00 28.10	CPS5
ATOM	3837	CA	ILE	15	12.439	28.378	55.972	1.00 27.56	CPS5
ATOM	3838	CB	ILE	15	13.916	28.640	55.587	1.00 28.43	CPS5
ATOM	3839	CG2		15	14.863	28.021	56.623	1.00 27.74	CPS5
ATOM	3840	CG1		15	14.201	28.042	54.204	1.00 26.73	CPS5
ATOM	3841	CD1		15	14.052	26.517	54.159	1.00 29.51	CPS5
ATOM	3842	С	ILE	15	12.226	28.739	57.441	1.00 29.85	CPS5
ATOM	3843	0	ILE	15	12.131	27.860	58.300	1.00 28.01	CPS5
ATOM	3844	N	ALA	16	12.145	30.039	57.724	1.00 30.25	CPS5
ATOM	3845	CA	ALA	16	11.929	30.508	59.097	1.00 31.84	CPS5
ATOM	3846	CB	ALA	16	11.937	32.038	59.142	1.00 31.96	CPS5
ATOM	3847	С	ALA	16	10.607	29.966	59.644	1.00 32.73	CPS5
ATOM	3848	0	ALA	16	10.534	29.550	60.802	1.00 33.57	CPS5
ATOM	3849	N	SER	17	9.564	29.958	58.820	1.00 33.10	CPS5
ATOM	3850	CA	SER	17	8.276	29.435	59.269	1.00 35.41	CPS5
ATOM	3851	CB	SER	17	7.206	29.639	58.201	1.00 36.49	CPS 5
ATOM	3852	OG	SER	17	6.988	31.024	57.990	1.00 40.91	CPS5
ATOM	3853	С	SER	17	8.369	27.954	59.617	1.00 35.50	CPS5
ATOM	3854	0	SER	17	7.938	27.532	60.696	1.00 35.16	CPS5
ATOM	3855	N	MET	18	8.927	27.164	58.705	1.00 35.27	CPS5
ATOM	3856	CA	MET	18	9.073	25.731	58.942	1.00 36.03	CPS5
ATOM	3857	CB	MET	18	9.701	25.045	57.726	1.00 36.24	CPS5
ATOM	3858	CG	MET	18	8.794	24.994	56.519	1.00 38.74	CPS 5
ATOM	3859	SD	MET	18	9.503	24.027	55.178	1.00 44.39	CPS5
ATOM	3860	CE	MET	18	10.534	25.241	54.428	1.00 38.98	CPS5
ATOM	3861	C	MET	18	9.918	25.462	60.180	1.00 35.92	CPS5
ATOM	3862	0	MET	18	9.597	24.580	60.979	1.00 37.63	CPS5
ATOM	3863	N	ALA	19	10.995	26.220	60.348	1.00 35.18	CPS5
ATOM ATOM	3864	CA	ALA	19	11.859	26.033	61.504	1.00 35.87	CPS5
ATOM	3865 3866	CB	ALA	19	13.081	26.932	61.401	1.00 35.73	CPS5
ATOM		С	ALA	19	11.087	26.348	62.783	1.00 38.24	CPS5
	3867	0	ALA	19	11.367	25.787	63.844	1.00 36.83	CPS5
ATOM	3868	N	GLY	20	10.106	27.239	62.669	1.00 38.64	CPS5
MOTA	3869	CA	GLY	20	9.320	27.619	63.827	1.00 40.77	CPS5
ATOM	3870	C	GLY	20	8.203	26.663	64.196	1.00 41.91	CPS5
	3871	0	GLY	20	7.826	26.580	65.361	1.00 43.62	CPS5
ATOM ATOM	3872	N	ARG	21	7.668	25.935	63.225	1.00 42.69	CPS5
	3873	CA	ARG	21	6.580	25.012	63.511	1.00 44.15	CPS 5
ATOM	3874	CB	ARG	21	5.574	25.026	62.362	1.00 46.42	CPS 5
ATOM	3875	CG	ARG	21	6.018	24.224	61.15 6	1.00 50.19	CPS5



SEP 0 9 2002

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0.S. FIG.	CLASS SUBCLASS	
APPROVED	à- en	DRAFTSMAH

3 0001									
ATOM	3876	CD	ARG	21	5.388	24.747	59.879	1.00 53.16	CPS5
ATOM	3877	NE	ARG	21	5.589	23.833	58.759	1.00 54.93	CPS5
ATOM	3878	CZ	ARG	21	5.372	24.159	57.490	1.00 56.47	CPS 5
ATOM	3879	NH1	ARG	21	4.956	25.383	57.184	1.00 57.16	CPS 5
ATOM	3880	NH2	ARG	21	5.554	23.258	56.533	1.00 56.82	CPS5
ATOM	3881	C	ARG	21	7.051	23.579	63.753	1.00 44.27	CPS5
ATOM	3882	ō	ARG	21	6.367	22.803	64.420	1.00 44.45	
ATOM	3883	N	GLN	22	8.213	23.226	63.209		CPS5
ATOM	3884	CA	GLN	22	8.741			1.00 42.85	CPS 5
ATOM	3885	CB	GLN			21.874	63.369	1.00 41.63	CPS5
				22	9.212	21.351	62.011	1.00 41.96	CPS5
ATOM	3886	CG	GLN	22	8.182	21.567	60.906	1.00 42.25	CPS5
ATOM	3887	CD	GLN	22	8.610	21.008	59.560	1.00 44.24	CPS5
ATOM	3888		GLN	22	7.988	21.293	58.533	1.00 45.66	CPS5
ATOM	3889	NE2		22	9.664	20.202	59.557	1.00 42.69	CPS5
ATOM	3890	С	GLN	22	9.882	21.862	64.387	1.00 41.06	CPS5
ATOM	3891	0	GLN	22	10.853	22.607	64.255	1.00 41.24	CPS5
ATOM	3892	N	LYS	23	9.764	20.995	65.390	1.00 39.60	CPS 5
ATOM	3893	CA	LYS	23	10.750	20.903	66.466	1.00 38.55	CPS5
ATOM	3894	CB	LYS	23	10.439	19.695	67.357	1.00 39.83	CPS 5
ATOM	3895	CG	LYS	23	11.370	19.589	68.551	1.00 41.79	
ATOM	3896	CD	LYS	23	10.771	18.745	69.654		CPS5
ATOM	3897	CE	LYS	23	10.448			1.00 43.79	CPS5
ATOM	3898	NZ	LYS	23		17.353	69.161	1.00 44.48	CPS 5
ATOM	3899				10.028	16.518	70.294	1.00 46.17	CPS 5
		С	LYS	23	12.236	20.885	66.106	1.00 37.06	CPS5
ATOM	3900	0	LYS	23	12.982	21.787	66.501	1.00 40.33	CPS5
ATOM	3901	N	ARG	24	12.679	19.862	65.389	1.00 32.83	CPS 5
ATOM	3902	CA	ARG	24	14.093	19.767	65.025	1.00 28.69	CPS5
ATOM	3903	CB	ARG	24	14.693	18.448	65.537	1.00 27.47	CPS5
ATOM	3904	CG	ARG	24	15.128	18.477	67.012	1.00 26.46	CPS 5
ATOM	3905	CD	ARG	24	15.742	17.141	67.435	1.00 26.25	CPS5
ATOM	3906	NE	ARG	24	14.723	16.093	67.528	1.00 26.94	CPS5
ATOM	3907	CZ	ARG	24	14.061	15.783	68.640	1.00 26.62	CPS5
ATOM	3908	NH1	ARG	24	14.304	16.423	69.781	1.00 28.42	CPS5
ATOM	3909	NH2		24	13.128	14.851	68.605	1.00 28.42	
ATOM	3910	C	ARG	24	14.269	19.874	63.519		CPS5
ATOM	3911	ō	ARG	24	14.863				CPS5
ATOM	3912	N	PHE	25		19.008	62.872	1.00 24.69	CPS5
ATOM	3913	CA	PHE	25	13.747	20.953	62.957	1.00 24.39	CPS5
ATOM	3914				13.848	21.148	61.515	1.00 24.06	CPS5
ATOM		CB	PHE	25	13.089	22.408	61.103	1.00 25.10	CPS5
ATOM	3915	CG	PHE	25	13.220	22.738	59.645	1.00 25.01	CPS5
	3916		PHE	25	14.065	23.754	59.224	1.00 26.44	CPS5
ATOM	3917	CD2	PHE	25	12.502	22.029	58.695	1.00 26.17	CPS5
ATOM	3918		PHE	25	14.192	24.063	57.867	1.00 26.84	CPS5
ATOM	3919		PHE	25	12.624	22.330	57.338	1.00 27.83	CPS5
ATOM	3920	cz	PHE	25	13.470	23.348	56.929	1.00 26.25	CPS5
ATOM	3921	С	PHE	25	15.289	21.241	61.034	1.00 23.02	CPS5
ATOM	3922	0	PHE	25	15.669	20.583	60.067	1.00 23.63	CPS5
ATOM	3923	N	ALA	26	16.096	22.055	61.702	1.00 21.62	CPS5
ATOM	3924	CA	ALA	26	17.481	22.211	61.272		
ATOM	3925	СВ	ALA	26	18.200			1.00 22.64	CPS5
ATOM	3926	c	ALA	26	18.200	23.213	62.171	1.00 21.17	CPS5
ATOM	3927	ō	ALA	26		20.868	61.295	1.00 22.18	CPS5
ATOM	3928	N			18.962	20.542	60.382	1.00 21.14	CPS5
ATOM			GLU	27	17.967	20.098	62.356	1.00 21.95	CPS5
	3929	CA	GLU	27	18.595	18.784	62.499	1.00 22.37	CPS5
ATOM	3930	CB	GLU	27	18.231	18.176	63.862	1.00 21.57	CPS5
ATOM	3931	CG	GLU	27	18.935	18.817	65.08 9	1.00 23.00	CPS5
ATOM	3932	CD	GLU	27	18.465	20.233	65.452	1.00 24.81	CPS5
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SEP 0 9 2002

TECH CENTER 1600/2900

	SHBOLAGE	200	
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ATOM	3933		GLU	27	17.353	20.647	65.056	1.00 23.58	CPS5
ATOM	3934	OE2	GLU	27	19.218	20.932	66.172	1.00 25.05	CPS5
ATOM	3935	С	GLU	27	18.184	17.831	61.369	1.00 23.57	CPS5
ATOM	3936	0	GLU	27	18.937	16.934	61.000	1.00 23.93	CPS5
MOTA	3937	N	ARG	28	16.981	18.015	60.833	1.00 23.21	CPS5
ATOM	3938	CA	ARG	28	16.502	17.173	59.742	1.00 25.30	CPS5
MOTA	3939	CB	ARG	28	14.995	17.391	59.530	1.00 28.97	CPS5
ATOM	3940	CG	ARG	28	14.413	16.636	58.327	1.00 31.14	CPS5
ATOM	3941	CD	ARG	28	12.911	16.353	58.503	1.00 35.90	CPS5
MOTA	3942	NE	ARG	28	12.063	17.535	58.340	1.00 36.29	CPS5
ATOM	3943	CZ	ARG	28	11.774	18.089	57.165	1.00 38.49	CPS5
ATOM	3944		ARG	28	12.264	17.571	56.045	1.00 37.03	CPS5
MOTA	3945	NH2	ARG	28	10.980	19.154	57.105	1.00 38.67	CPS5
ATOM	3946	С	ARG	28	17.245	17.488	58.439	1.00 24.41	CPS5
MOTA	3947	0	ARG	28	17.582	16.596	57.666	1.00 24.06	CPS5
ATOM	3948	N	ILE	29	17.517	18.765	58.218	1.00 23.36	CPS5
ATOM	3949	CA	ILE	29	18.183	19.212	56.997	1.00 24.49	CPS5
ATOM	3950	CB	ILE	29	17.817	20.693	56.704	1.00 24.90	CPS5
ATOM	3951		ILE	29	18.374	21.123	55.334	1.00 26.73	CPS5
ATOM	3952		ILE	29	16.305	20.880	56.773	1.00 24.80	CPS5
MOTA	3953		ILE	29	15.527	19.982	55.843	1.00 23.16	CPS5
ATOM	3954	С	ILE	29	19.708	19.121	56.983	1.00 24.05	CPS5
ATOM	3955	0	ILE	29	20.313	18.817	55.949	1.00 23.72	CPS5
ATOM	3956	N	LEU	30	20.323	19.383	58.132	1.00 23.56	CPS5
ATOM	3957	CA	LEU	30	21.778	19.444	58.240	1.00 23.33	CPS5
ATOM	3958	CB	LEU	30	22.151	20.701	59.035	1.00 22.47	CPS5
ATOM	3959	CG	LEU	30	21.503	22.020	58.591	1.00 23.18	CPS5
ATOM	3960		LEU	30	21.940	23.141	59.519	1.00 23.77	CPS5
ATOM	3961		LEU	30	21.901	22.348	57.157	1.00 22.19	CPS5
ATOM	3962	С	LEU	30	22.492	18.238	58.854	1.00 24.18	CPS5
ATOM	3963	0	LEU	30	21.966	17.577	59.753	1.00 24.62	CPS5
ATOM	3964	N	THR	31	23.704	17.976	58.363	1.00 24.03	CPS5
ATOM	3965	CA	THR	31	24.531	16.878	58.862	1.00 24.72	CPS5
ATOM	3966	CB	THR	31	25.626	16.494	57.850	1.00 25.78	CPS5
ATOM ATOM	3967 3968		THR	31	26.575	17.563	57.761	1.00 26.99	CPS5
ATOM			THR	31	25.022	16.234	56.466	1.00 24.96	CPS5
ATOM	3969 3970	C	THR	31	25.228	17.351	60.140	1.00 24.37	CPS5
ATOM	3971	N	ARG	31 32	25.134	18.520	60.514	1.00 24.09	CPS5
ATOM	3971	CA	ARG	32	25.943	16.452	60.806	1.00 25.54	CPS5
ATOM	3973	CB	ARG	32	26.642	16.832	62.031	1.00 27.17	CPS5
ATOM	3974	CG	ARG	32	27.429 26.583	15.651	62.590	1.00 28.99	CPS5
ATOM	3975	CD	ARG	32	27.476	14.597	63.261	1.00 31.34	CPS5
ATOM	3976	NE	ARG	32	26.701	13.684	64.109	1.00 34.50	CPS5
ATOM	3977	CZ	ARG	32	27.200	12.698 11.916	64.853 65.809	1.00 38.58	CPS5
ATOM	3978		ARG	32	26.419	11.916	66.435		CPS5
ATOM	3979		ARG	32	28.480	12.009	66.145	1.00 37.96 1.00 42.21	CPS5 CPS5
ATOM	3980	C	ARG	32	27.589	18.014	61.865	1.00 42.21	CPS5
ATOM	3981	ō	ARG	32	27.562	18.940	62.666	1.00 27.70	CPS5
ATOM	3982	N	SER	33	28.439	17.987	60.841	1.00 28.37	CPS5
ATOM	3983	CA	SER	33	29.379	19.088	60.652	1.00 27.37	CPS5
ATOM	3984	CB	SER	33	30.397	18.746	59.556	1.00 28.23	CPS5
ATOM	3985	OG	SER	33	29.759	18.525	58.309	1.00 30.14	CPS5
ATOM	3986	c	SER	33	28.661	20.398	60.330	1.00 34.75	CPS5
ATOM	3987	ŏ	SER	33	29.082	21.464	60.776	1.00 27.70	CPS5
ATOM	3988	N	GLU	34	27.578	20.319	59.560	1.00 27.19	CPS5
ATOM	3989	CA	GLU	34	26.804	21.511	59.212	1.00 27.23	CPS5
					20.004	-1.511	33.212	1.00 27.47	Cros



RECEIVED SEP 0 9 2002

FIG. 1A-70

TECH CENTER 1600/2900

. F1G.	SS SUBCLASS	
APPROVED 5.0	67 (1.4.55	DRAFTSMAH

ATOM	3990	CB		34	25.759	21.171	58.148	1.00 27.07	CPS5
ATOM	3991	CG	GLU	34	26.368	20.872	56.783	1.00 28.76	CPS5
ATOM	3992	CD	GLU	34	25.376	20.290	55.782	1.00 28.74	CPS5
ATOM	3993	OE	1 GLU	34	25.664	20.350	54.569	1.00 31.36	CPS5
ATOM	3994	OE	2 GLU	34	24.320	19.764	56.192	1.00 26.92	CPS5
ATOM	3995	С	GLU	34	26.121	22.080	60.454	1.00 27.58	CPS5
ATOM	3996	0	GLU	34	26.028	23.300	60.624	1.00 26.80	
ATOM	3997	N	LEU	35	25.629	21.196	61.319	1.00 26.86	CPS5
ATOM	3998	CA	LEU	35	24.988	21.653	62.545	1.00 27.86	CPS5
ATOM	3999	CB	LEU	35	24.322	20.476	63.272	1.00 26.37	CPS5
ATOM	4000	CG	LEU	35	23.004	19.992	62.650	1.00 26.60	CPS5
ATOM	4001		1 LEU	35	22.597	18.649	63.255	1.00 25.80	CPS5
ATOM	4002		2 LEU	35	21.906	21.050	62.890	1.00 27.30	CPS5
ATOM	4003	С	LEU	35	26.032	22.333	63.442	1.00 28.95	CPS5
ATOM	4004	0	LEU	35	25.727	23.317	64.104	1.00 28.95	CPS5
ATOM	4005	N	ASP	36	27.264	21.825	63.458	1.00 29.27	CPS5
ATOM	4006	CA	ASP	36	28.306	22.453	64.279	1.00 31.26	CPS5
ATOM	4007	CB	ASP	36	29.649	21.740	64.127		CPS5
ATOM	4008	CG	ASP	36	29.668	20.386	64.795	1.00 36.86	CPS5
ATOM	4009	ODI	LASP	36	28.990	20.235		1.00 39.66	CPS5
ATOM	4010		2 ASP	36	30.373	19.479	65.833	1.00 43.45	CPS5
ATOM	4011	С	ASP	36	28.481	23.905	64.297	1.00 41.30	CPS5
ATOM	4012	ō	ASP	36	28.608	24.794	63.871	1.00 34.39	CPS5
ATOM	4013	N	GLN	37	28.488	24.140	64.722	1.00 34.60	CPS5
ATOM	4014	CA	GLN	37	28.639	25.483	62.563 62.015	1.00 33.83	CPS5
ATOM	4015	CB	GLN	37	28.809	25.394		1.00 35.12	CPS5
ATOM	4016	CG	GLN	37	30.079	24.660	60.499	1.00 36.30	CPS5
ATOM	4017	CD	GLN	37	29.944	24.026	60.055	1.00 41.36	CPS5
ATOM	4018		GLN	37	29.434	24.646	58.676	1.00 43.00	CPS5
ATOM	4019		GLN	37	30.408		57.746	1.00 44.80	CPS5
ATOM	4020	C	GLN	37	27.409	22.786	58.541	1.00 44.26	CPS5
ATOM	4021	0	GLN	37	27.513	26.328 27.470	62.344	1.00 34.18	CPS5
ATOM	4022	N	TYR	38	26.240	25.736	62.794 62.126	1.00 33.82	CPS5
ATOM	4023	CA	TYR	38	24.963	26.395		1.00 32.84	CPS5
ATOM	4024	CB	TYR	38	23.846	25.419	62.349	1.00 32.66	CPS5
ATOM	4025	CG	TYR	38	22.433	25.884	61.961 62.224	1.00 29.71	CPS5
ATOM	4026	CD1	TYR	38	21.721	25.404		1.00 29.29	CPS5
ATOM	4027		TYR	38	20.401	25.776	63.317 63.541	1.00 29.80	CPS5
ATOM	4028	CD2		38	21.788	26.763		1.00 31.00	CPS5
ATOM	4029	CE2		38	20.459	27.146	61.355	1.00 28.96	CPS5
ATOM	4030	CZ	TYR	38	19.776	26.644	61.571	1.00 28.65	CPS5
ATOM	4031	ОН	TYR	38	18.462	26.985	62.665	1.00 29.30	CPS5
ATOM	4032	С	TYR	38	24.746	26.939	62.885 63.765	1.00 28.92	CPS5
ATOM	4033	0	TYR	38	24.292	28.068	63.765	1.00 34.02	CPS5
ATOM	4034	N	TYR	39	25.076	26.154	64.780	1.00 34.37	CPS5
ATOM	4035	CA	TYR	39	24.860	26.613		1.00 36.23	CPS5
ATOM	4036	CB	TYR	39	24.762	25.414	66.144	1.00 38.88	CPS5
ATOM	4037	CG	TYR	39	23.371	24.847	67.082	1.00 38.30	CPS5
ATOM	4038		TYR	39	22.273		67.036	1.00 38.06	CPS5
ATOM	4039		TYR	39	20.974	25.658 25.194	67.338 67.203	1.00 38.93	CPS5
ATOM	4040		TYR	39	23.134			1.00 39.58	CPS5
ATOM	4041			39	21.837	23.546	66.608	1.00 37.49	CPS5
ATOM	4042	cz	TYR	39	20.760	23.064	66.469	1.00 37.88	CPS5
ATOM	4043	ОН	TYR	39		23.893	66.763	1.00 39.42	CPS5
ATOM	4044	c	TYR	39	19.470	23.450	66.592	1.00 38.55	CPS5
ATOM	4045	ō	TYR	39	25.816	27.658	66.692	1.00 41.19	CPS5
ATOM	4046	N	GLU	40	25.662 26.789	28.109	67.822	1.00 42.90	CPS5
			220	40	26.789	28.060	65.887	1.00 43.80	CPS5



SEP 0 9 2002 TECH CENTER 1600/2900



MOTA	4047	CA	GLU	40	27.731	29.090	66.304	1.00 46.08	CPS5
ATOM	4048	CB	GLU	40	29.140	28.737	65.834	1.00 48.41	CPS5
ATOM	4049	CG	GLU	40	29.806	27.639	66.639	1.00 52.50	CPS5
ATOM	4050	CD	GLU	40	31.155	27.248	66.063	1.00 54.95	CPS5
ATOM	4051	OE1	GLU	40	31.969	28.154	65.774	1.00 56.23	CPS5
MOTA	4052	OE2	GLU	40	31.403	26.033	65.904	1.00 57.17	CPS5
ATOM		C	GLU	40	27.322	30.446	65.721	1.00 46.24	CPS5
ATOM		0	GLU	40	27.932	31.475	66.023	1.00 46.47	CPS5
ATOM		N	LEU	41	26.279	30.443	64.896	1.00 45.08	
ATOM		CA	LEU	41	25.803	31.664	64.254	1.00 44.90	CPS5
ATOM		CB	LEU	41	25.304	31.348	62.840		CPS5
ATOM		CG	LEU	41	26.227	30.623	61.859	1.00 44.02	CPS5
ATOM			LEU	41	25.443			1.00 43.61	CPS5
ATOM			LEU	41		30.306	60.591	1.00 42.67	CPS5
ATOM		CD2	LEU		27.439	31.480	61.530	1.00 43.84	CPS5
ATOM		0	LEU	41	24.685	32.376	65.013	1.00 45.61	CPS5
				41	24.021	31.789	65.869	1.00 45.79	CPS5
ATOM		N	SER	42	24.479	33.648	64.677	1.00 46.42	CPS5
ATOM		CA	SER	42	23.432	34.456	65.288	1.00 47.43	CPS5
ATOM		CB	SER	42	23.615	35.924	64.915	1.00 48.22	CPS5
ATOM		OG	SER	42	23.440	36.106	63.520	1.00 48.72	CPS5
ATOM		C	SER	42	22.105	33.963	64.734	1.00 47.92	CPS5
ATOM		0	SER	42	22.081	33.205	63.763	1.00 47.71	CPS5
ATOM		N	GLU	43	21.000	34.399	65.328	1.00 48.18	CPS5
ATOM		CA	GLU	43	19.689	33.959	64.861	1.00 48.69	CPS5
ATOM		CB	GLU	43	18.581	34.563	65.728	1.00 50.88	CPS5
ATOM		CG	GLU	43	17.286	33.765	65.683	1.00 53.85	CPS5
ATOM		CD	GLU	43	16.099	34.579	65.201	1.00 56.30	CPS5
ATOM			GLU	43	16.189	35.176	64.105	1.00 57.99	CPS5
ATOM		OE2	GLU	43	15.073	34.614	65.916	1.00 56.86	CPS5
ATOM	4076	C	GLU	43	19.449	34.308	63.389	1.00 47.59	CPS5
MOTA		0	GLU	43	18.899	33.503	62.635	1.00 46.68	CPS5
MOTA	4078	N	LYS	44	19.861	35.504	62.979	1.00 46.55	CPS5
ATOM	4079	CA	LYS	44	19.680	35.926	61.591	1.00 46.07	CPS5
ATOM	4080	CB	LYS	44	19.973	37.422	61.439	1.00 47.29	CPS5
ATOM	4081	CG	LYS	44	19.730	37.935	60.031	1.00 49.35	CPS5
ATOM	4082	CD	LYS	44	20.148	39.384	59.857	1.00 50.89	CPS5
ATOM	4083	CE	LYS	44	19.837	39.855	58.440	1.00 52.29	CPS5
ATOM	4084	NZ	LYS	44	20.265	41.261	58.188	1.00 53.26	CPS5
ATOM	4085	С	LYS	44	20.597	35.130	60.660	1.00 44.52	CPS5
ATOM	4086	0	LYS	44	20.185	34.698	59.579	1.00 43.62	CPS5
ATOM	4087	N	ARG	4.5	21.842	34.944	61.084	1.00 42.61	CPS5
ATOM	4088	CA	ARG	45	22.816	34.195	60.297	1.00 41.42	CPS5
ATOM	4089	CB	ARG	4.5	24.193	34.284	60.957	1.00 43.69	CPS5
ATOM	4090	CG	ARG	4.5	25.001	35.512	60.552	1.00 47.18	CPS5
ATOM	4091	CD	ARG	45	26.039	35.120	59.517	1.00 50.46	CPS5
ATOM	4092	NE	ARG	45	25.455	34.243	58.506	1.00 53.21	CPS5
ATOM	4093	CZ	ARG	45	26.141	33.355	57.794	1.00 54.22	CPS5
ATOM	4094		ARG	45	27.450	33.219	57.975	1.00 54.22	
ATOM	4095	NH2		45	25.514	32.593			CPS5
ATOM	4096	C	ARG	45	22.385		56.909	1.00 54.37	CPS5
ATOM	4097	ō	ARG	45	22.620	32.735	60.156	1.00 39.25	CPS5
ATOM	4098	N	LYS	46		32.100	59.128	1.00 37.24	CPS5
ATOM	4099	CA	LYS	46	21.748	32.209	61.196	1.00 36.43	CPS5
ATOM	4100	CB	LYS	46	21.273	30.830	61.175	1.00 34.18	CPS 5
ATOM	4101	CG	LYS	46	20.618	30.472	62.511	1.00 34.58	CPS5
ATOM	4102	CD	LYS	46	21.608	30.164	63.630	1.00 35.23	CPS5
ATOM	4102	CE	LYS		20.871	29.751	64.894	1.00 37.58	CPS5
-11011	.103	CE	D13	46	21.842	29.392	66.010	1.00 39.36	CPS5

SEP 0 9 2002

TECH CENTER 1600/2900



FIG. 1A-72

	SUBCI ASS	
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ATOM	4104	NZ	LYS	46	21.100	29.022	67.241	1.00 40.50	CPS5
ATOM	4105	С	LYS	46	20.267	30.612	60.047	1.00 33.30	CPS5
ATOM	4106	0	LYS	46	20.350	29.631	59.310	1.00 31.70	CPS5
ATOM	4107	N	ASN	47	19.313	31.531	59.924	1.00 31.25	CPS5
ATOM	4108	CA	ASN	47	18.295	31.424	58.892	1.00 30.79	CPS5
ATOM	4109	CB	ASN	47	17.298	32.575	59.020	1.00 32.61	CPS5
ATOM	4110	CG	ASN	47	16.216	32.532	57.963	1.00 33.88	CPS5
ATOM	4111		1 ASN	47	15.427	31.588	57.896	1.00 34.99	CPS5
ATOM	4112	ND:		47	16.176	33.558	57.121	1.00 36.56	CPS5
ATOM	4113	C	ASN	47	18.944	31.440	57.513	1.00 31.05	CPS5
ATOM	4114	0	ASN	47	18.588	30.637	56.648	1.00 30.48	CPS5
ATOM	4115	N	GLU	48	19.888	32.358	57.311	1.00 28.97	CPS5
ATOM	4116	CA	GLU	48	20.588	32.468	56.031	1.00 29.63	CPS5
ATOM	4117	CB	GLU	48	21.570	33.640	56.061	1.00 31.86	CPS5
ATOM	4118	CG	GLU	48	20.921	34.975	56.372	1.00 37.62	CPS5
ATOM	4119	CD	GLU	48	21.936	36.092	56.540	1.00 40.25	CPS5
ATOM	4120		CLU	48	21.525	37.217	56.898	1.00 42.86	CPS5
ATOM	4121	OE:		48	23.141	35.845	56.313	1.00 41.40	CPS5
ATOM	4122	C	GLU	48	21.358	31.187	55.726	1.00 27.51	CPS5
ATOM ATOM	4123	0	GLU	48	21.281	30.644	54.622	1.00 26.82	CPS5
ATOM	4124	N	PHE	49	22.106	30.712	56.711	1.00 25.07	CPS5
ATOM	4125	CA	PHE	49	22.886	29.497	56.552	1.00 25.50	CPS5
ATOM	4126 4127	CB	PHE	49	23.636	29.194	57.844	1.00 25.32	CPS5
ATOM	4128		PHE.	49	24.519	27.986	57.765	1.00 26.38	CPS 5
ATOM	4129		PHE	49	25.798	28.077	57.233	1.00 27.15	CPS 5
ATOM	4130	CE1		49	24.080	26.757	58.249	1.00 24.90	CPS5
ATOM	4131	CE2		49	26.640	26.954	57.189	1.00 28.06	CPS5
ATOM	4132	CZ	PHE	49	24.903	25.635	58.211	1.00 25.87	CPS5
ATOM	4133	c	PHE	49 49	26.195	25.736	57.678	1.00 26.35	CPS5
ATOM	4134	0	PHE	49	21.991	28.312	56.203	1.00 24.96	CPS5
ATOM	4135	N	LEU	50	22.255	27.581	55.248	1.00 24.24	CPS5
ATOM	4136	CA	LEU	50	20.939	28.114	56.995	1.00 23.68	CPS 5
ATOM	4137	CB	LEU	50	18.974	27.005	56.773	1.00 23.00	CPS5
ATOM	4138	CG	LEU	50	17.860	26.962 25.903	57.892	1.00 24.58	CPS5
ATOM	4139		LEU	50	18.431		57.864	1.00 24.45	CPS 5
ATOM	4140		LEU	50	17.022	24.483 26.072	57.785	1.00 24.94	CPS5
ATOM	4141	C	LEU	50	19.349	27.082	59.142 55.403	1.00 23.53	CPS 5
ATOM	4142	ō	LEU	50	19.268	26.083		1.00 22.61	CPS 5
ATOM	4143	N	ALA	51	18.865	28.260	54.693 55.021	1.00 21.59	CPS5
ATOM	4144	CA	ALA	51	18.213	28.390	53.723	1.00 21.89	CPS5
ATOM	4145	CB	ALA	51	17.637	29.799	53.725	1.00 21.84 1.00 21.05	CPS5
ATOM	4146	C	ALA	51	19.191	28.076	52.585	1.00 21.05	CPS5 CPS5
ATOM	4147	0	ALA	51	18.813	27.458	51.587	1.00 21.23	
ATOM	4148	N	GLY	52	20.442	28.506	52.734	1.00 21.20	CPS5 CPS5
ATOM	4149	CA	GLY	52	21.437	28.245	51.700	1.00 21.20	CPS5
ATOM	4150	С	GLY	52	21.769	26.767	51.563	1.00 22.06	CPS5
ATOM	4151	0	GLY	52	21.929	26.252	50.452	1.00 20.70	CPS5
ATOM	4152	N	ARG	53	21.888	26.074	52.693	1.00 21.88	CPS5
ATOM	4153	CA	ARG	53	22.188	24.645	52.659	1.00 21.58	CPS5
ATOM	4154	CB	ARG	53	22.565	24.152	54.065	1.00 23.65	CPS5
ATOM	4155	CG	ARG	53	24.066	24.127	54.329	1.00 27.20	CPS5
ATOM	4156	CD	ARG	53	24.751	25.409	53.912	1.00 30.18	CPS5
ATOM	4157	NE	ARG	53	26.181	25.365	54.194	1.00 32.58	CPS5
ATOM	4158	CZ	ARG	53	27.072	26.204	53.677	1.00 35.33	CPS5
ATOM	4159	NH1		53	26.690	27.163	52.836	1.00 37.77	CPS5
ATOM	4160	NH2	ARG	53	28.350	26.089	54.006	1.00 37.90	CPS5



SEP 0 9 2002

FIG. 1A-73

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MOTA	4161	C	ARG	53	20.976	23.890	52.125	1.00 21.40	CPS5
ATOM	4162	0	ARG	53	21.106	22.921	51.365	1.00 20.53	CPS5
MOTA	4163	N	PHE	54	19.795	24.341	52.528	1.00 19.73	CPS5
ATOM	4164	CA	PHE	54	18.548	23.745	52.070	1.00 19.35	CPS5
ATOM	4165	CB	PHE	54	17.364	24.482	52.724	1.00 19.38	CPS5
ATOM	4166	CG	PHE	54	16.023	23.926	52.353	1.00 20.72	CPS5
ATOM	4167	CD1	PHE	54	15.330	24.414	51.245	1.00 22.15	CPS5
ATOM	4168	CD2	PHE	54	15.448	22.903	53.107	1.00 21.41	CPS5
ATOM	4169	CE1	PHE	54	14.080	23.891	50.893	1.00 22.91	CPS5
ATOM	4170	CE2	PHE	54	14.196	22.371	52.762	1.00 22.41	CPS5
ATOM	4171	CZ	PHE	54	13.513	22.868	51.654	1.00 22.38	CPS5
ATOM	4172	C	PHE	54	18.484	23.873	50.537	1.00 19.62	CPS5
ATOM	4173	0	PHE	54	18.223	22.901	49.821	1.00 18.89	CPS5
ATOM	4174	N	ALA	55	18.736	25.082	50.046	1.00 19.98	CPS5
ATOM	4175	CA	ALA	55	18.690	25.348	48.608	1.00 19.92	CPS5
ATOM	4176	CB	ALA	55	18.930	26.839	48.347	1.00 18.81	CPS5
ATOM	4177	C	ALA	55	19.721	24.515	47.859	1.00 19.28	CPS5
ATOM	4178	0	ALA	55	19.442	23.972	46.788	1.00 19.25	CPS5
MOTA	4179	N	ALA	56	20.916	24.398	48.422	1.00 19.74	CPS5
ATOM	4180	CA	ALA	56	21.954	23.621	47.755	1.00 20.82	CPS5
MOTA	4181	CB	ALA	56	23.299	23.838	48.446	1.00 20.78	CPS5
ATOM	4182	С	ALA	56	21.622	22.130	47.693	1.00 20.48	CPS5
ATOM	4183	0	ALA	56	21.944	21.459	46.702	1.00 20.22	CPS5
MOTA	4184	N	LYS	57	20.993	21.600	48.746	1.00 19.44	CPS5
ATOM	4185	CA	LYS	57	20.642	20.187	48.754	1.00 19.12	CPS5
ATOM	4186	CB	LYS	57	20.336	19.718	50.191	1.00 18.95	CPS5
ATOM	4187	CG	LYS	57	21.571	19.809	51.077	1.00 18.78	CPS5
ATOM	4188	CD	LYS	57	21.395	19.116	52.429	1.00 22.43	CPS5
ATOM	4189	CE	LYS	57	22.575	19.458	53.329	1.00 22.68	CPS5
ATOM	4190	NZ	LYS	57	22.712	18.541	54.502	1.00 21.60	CPS5
ATOM	4191	С	LYS	57	19.465	19.937	47.821	1.00 20.77	CPS5
ATOM	4192	0	LYS	57	19.401	18.900	47.160	1.00 20.15	CPS5
ATOM	4193	N	GLU	58	18.535	20.885	47.757	1.00 19.45	CPS5
MOTA	4194	CA	GLU	58	17.410	20.738	46.845	1.00 21.16	CPS5
MOTA	4195	CB	GLU	58	16.409	21.887	47.020	1.00 21.14	CPS5
ATOM	4196	CG	GLU	58	15.520	21.769	48.247	1.00 25.24	CPS5
ATOM	4197	CD	GLU	58	14.558	20.605	48.153	1.00 29.18	CPS5
ATOM	4198		GLU	58	14.482	19.993	47.066	1.00 31.68	CPS5
ATOM	4199		GLU	58	13.875	20.305	49.156	1.00 29.87	CPS5
ATOM	4200	C	GLU	58	17.943	20.741	45.410	1.00 20.35	CPS5
MOTA	4201	0	GLU	58	17.543	19.908	44.590	1.00 20.00	CPS5
MOTA	4202	N	ALA	59	18.848	21.675	45.113	1.00 20.46	CPS5
ATOM	4203	CA	ALA	59	19.418	21.765	43.769	1.00 20.45	CPS5
ATOM	4204	CB	ALA	59	20.353	22.971	43.655	1.00 20.63	CPS5
ATOM	4205	C	ALA	59	20.175	20.489	43'. 436	1.00 20.79	CPS5
ATOM	4206	0	ALA	59	20.104	19.985	42.312	1.00 20.80	CPS5
MOTA	4207	N	PHE	60	20.916	19.965	44.404	1.00 19.71	CPS5
ATOM	4208	CA	PHE	60	21.643	18.730	44.153	1.00 19.50	CPS5
ATOM	4209	CB	PHE	60	22.511	18.349	45.361	1.00 20.28	CPS5
MOTA	4210	CG	PHE	60	23.252	17.057	45.172	1.00 22.22	CPS5
MOTA	4211		PHE	60	24.498	17.034	44.548	1.00 22.07	CPS5
ATOM	4212		PHE	60	22.657	15.850	45.538	1.00 23.50	CPS5
ATOM	4213		PHE	60	25.145	15.810	44.285	1.00 25.08	CPS5
ATOM	4214		PHE	60	23.287	14.629	45.282	1.00 26.22	CPS5
ATOM ATOM	4215	cz	PHE	60	24.534	14.614	44.652	1.00 24.97	CPS5
ATOM	4216	C	PHE	60	20.665	17.588	43.857	1.00 19.97	CPS5
AIOM	4217	0	PHE	60	20.893	16.774	42.946	1.00 20.76	CPS5



SEP 0 9 2002

TECH CENTER 1600/2900

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MOTA	4218	N	SER	61	19.575	17.530	44.615	1.00 19.93
ATOM	4219	CA	SER	61	18.596	16.461	44.437	1.00 22.05
ATOM	4220	CB	SER	61	17.542	16.505	45.550	1.00 21.89
ATOM	4221	OG	SER	61	16.571	17.505	45.308	1.00 22.40
ATOM	4222	С	SER	61	17.931	16.519	43.067	1.00 22.70
ATOM	4223	0	SER	61	17.482	15.494	42.540	1.00 23.10
ATOM	4224	N	LYS	62	17.874	17.716	42.487	1.00 21.75
ATOM	4225	CA	LYS	62	17.292	17.888	41.158	1.00 22.11
ATOM	4226	CB	LYS	62	16.914	19.349	40.932	1.00 23.25
ATOM	4227	CG	LYS	62	15.636	19.790	41.661	1.00 26.97
ATOM	4228	CD	LYS	62	15.515	21.316	41.597	1.00 29.60
ATOM	4229	CE	LYS	62	14.085	21.787	41.383	1.00 29.60
ATOM	4230	NZ	LYS	62	13.174	21.402	42.470	1.00 35.09
ATOM	4231	С	LYS	62	18.290	17.431	40.095	1.00 22.61
ATOM	4232	0	LYS	62	17.897	16.841	39.079	1.00 22.61
ATOM	4233	N	ALA	63	19.577	17.695	40.333	1.00 21.05
MOTA	4234	CA	ALA	63	20.627	17.283	39.408	1.00 21.03
ATOM	4235	CB	ALA	63	21.965	17.909	39.801	1.00 21.40
ATOM	4236	С	ALA	63	20.737	15.767	39.476	1.00 23.26
ATOM	4237	0	ALA	63	21.006	15.113	38.473	1.00 23.26
ATOM	4238	N	PHE	64	20.525	15.225	40.672	1.00 23.91
ATOM	4239	CA	PHE	64	20.591	13.782	40.916	1.00 25.22
MOTA	4240	CB	PHE	64	20.463	13.512	42.419	1.00 24.79
ATOM	4241	CG	PHE	64	20.781	12.097	42.818	1.00 24.79
ATOM	4242	CD1	PHE	64	22.094	11.642	42.822	1.00 27.22
ATOM	4243		PHE	64	19.768	11.233	43.217	1.00 27.62
ATOM	4244		PHE	64	22.398	10.343	43.224	1.00 27.62
ATOM	4245	CE2	PHE	64	20.061	9.931	43.622	1.00 28.83
ATOM	4246	CZ	PHE	64	21.377	9.489	43.625	1.00 28.53
ATOM	4247	С	PHE	64	19.453	13.109	40.147	1.00 26.39
ATOM	4248	0	PHE	64	19.554	11.941	39.766	1.00 28.07
ATOM	4249	N	GLY	65	18.381	13.862	39.911	1.00 26.10
ATOM	4250	CA	GLY	65	17.251	13.368	39.143	1.00 27.17
ATOM	4251	С	GLY	65	16.088	12.768	39.905	1.00 28.46
ATOM	4252	0	GLY	65	15.117	12.317	39.298	1.00 28.55
ATOM	4253	N	THR	66	16.157	12.789	41.231	1.00 28.12
ATOM	4254	CA	THR	66	15.099	12.191	42.037	1.00 29.33
ATOM	4255	CB	THR	66	15.663	11.062	42.903	1.00 29.96
ATOM	4256	OG1	THR	66	16.635	11.608	43.804	1.00 29.92
ATOM	4257	CG2	THR	66	16.326	10.009	42.038	1.00 30.68
ATOM	4258	C	THR	66	14.410	13.148	42.984	1.00 28.71
ATOM	4259	0	THR	66	13.269	12.915	43.378	1.00 28.56
ATOM	4260	N	GLY	67	15.098	14.227	43.343	1.00 27.58
ATOM	4261	CA	GLY	67	14.530	15.150	44.305	1.00 27.06
ATOM	4262	С	GLY	67	14.741	14.479	45.657	1.00 27.43
ATOM	4263	0	GLY	6 7	15.278	13.367	45.712	1.00 26.28
ATOM	4264	N	ILE	68	14.343	15.145	46.737	1.00 26.71
ATOM	4265	CA	ILE	68	14.491	14.593	48.082	1.00 28.68
ATOM	4266	CB	ILE	68	14.470	15.715	49.166	1.00 27.25
ATOM	4267	CG2	ILE	68	14.574	15.098	50.569	1.00 27.25
MOTA	4268	CG1	ILE	68	15.630	16.697	48.936	1.00 24.63
ATOM	4269	CD1	ILE	68	17.030	16.084	49.112	1.00 23.40
ATOM	4270	С	ILE	68	13.335	13.629	48.342	1.00 30.86
ATOM	4271	0	ILE	68	12.167	13.982	48.169	1.00 31.01
MOTA	4272	N	GLY	69	13.671	12.412	48.752	1.00 33.01
MOTA	4273	CA	GLY	69	12.654	11.415	49.022	1.00 34.73
ATOM	4274	C	GLY	69	13.291	10.115	49.470	1.00 36.57

FIG. 1A-74



SEP 0 9 2002

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TECH CENTER 1600/2900



ATOM	4275	0	GLY	69	14.363	10.112	50.079	1.00 36.27	CPS5
ATOM	4276	N	ARG	70	12.653	8.997	49.152	1.00 38.18	CPS5
ATOM	4277	CA	ARG	70	13.203	7.724	49.579	1.00 39.66	CPS5
ATOM	4278	CB	ARG	70	12.137	6.627	49.493	1.00 43.12	CPS5
ATOM	4279	CG	ARG	70	11.182	6.661	50.696	1.00 47.23	CPS5
ATOM	4280	CD	ARG	70	11.972	6.780	52.019	1.00 49.65	CPS5
ATOM	4281	NE	ARG	70	11.469	7.858	52.870	1.00 51.86	CPS5
ATOM	4282	CZ	ARG	70	12.239	8.672	53.590	1.00 52.77	CPS5
ATOM	4283	NH1	ARG	70	13.558	8.540	53.569	1.00 53.05	CPS5
ATOM	4284	NH2	ARG	70	11.691	9.627	54.328	1.00 52.96	CPS5
ATOM	4285	С	ARG	70	14.468	7.317	48.855	1.00 37.80	CPS5
ATOM	4286	0	ARG	70	15.221	6.478	49.345	1.00 37.07	CPS5
ATOM	4287	N	GLN	71	14.726	7.926	47.703	1.00 36.29	CPS5
ATOM	4288	CA	GLN	71	15.932	7.598	46.959	1.00 35.22	CPS5
ATOM	4289	CB	GLN	71	15.707	7.778	45.453	1.00 36.48	CPS5
ATOM	4290	CG	GLN	71	14.534	6.985	44.889	1.00 38.95	CPS5
ATOM	4291	CD	GLN	71	14.402	7.129	43.379	1.00 40.20	CPS5
MOTA	4292	OE1	GLN	71	15.236	6.631	42.622	1.00 40.67	CPS5
ATOM	4293	NE2	GLN	71	13.355	7.827	42.937	1.00 40.72	CPS5
ATOM	4294	C	GLN	71	17.084	8.483	47.412	1.00 33.38	CPS5
ATOM	4295	0	GLN	71	18.248	8.110	47.276	1.00 33.43	CPS5
ATOM	4296	N	LEU	72	16.759	9.650	47.966	1.00 30.70	CPS5
ATOM	4297	CA	LEU	72	17.786	10.591	48.409	1.00 27.96	CPS5
ATOM	4298	CB	LEU	72	18.204	11.478	47.231	1.00 26.31	CPS5
ATOM	4299	CG	LEU	72	19.285	12.532	47.448	1.00 26.21	CPS5
ATOM	4300	CD1	LEU	72	20.626	11.867	47.673	1.00 27.19	CPS 5
ATOM	4301	CD2	LEU	72	19.338	13.446	46.213	1.00 25.53	CPS5
ATOM	4302	С	LEU	72	17.279	11.469	49.556	1.00 27.62	CPS5
ATOM	4303	0	LEU	72	16.203	12.070	49.470	1.00 27.05	CPS5
ATOM	4304	N	SER	73	18.076	11.545	50.616	1.00 26.31	CPS5
ATOM	4305	CA	SER	73	17.735	12.323	51.805	1.00 25.42	CPS5
ATOM	4306	CB	SER	73	17.889	11.441	53.051	1.00 26.75	CPS5
ATOM	4307	OG	SER	73	17.970	12.228	54.231	1.00 27.96	CPS5
ATOM	4308	С	SER	73	18.633	13.539	51.965	1.00 24.08	CPS5
ATOM	4309	0	SER	73	19.733	13.581	51.419	1.00 23.91	CPS5
ATOM	4310	N	PHE	74	18.165	14.525	52.721	1.00 23.49	CPS5
ATOM	4311	CA	PHE	74	18.975	15.707	52.995	1.00 23.97	CPS5
ATOM	4312	CB	PHE	74	18.246	16.657	53.955	1.00 24.68	CPS5
ATOM	4313	CG	PHE	74	17.124	17.430	53.319	1.00 25.48	CPS5
ATOM	4314		PHE	74	17.392	18.421	52.371	1.00 26.10	CPS5
ATOM	4315		PHE	74	15.801	17.176	53.672	1.00 26.28	CPS5
ATOM	4316		PHE	74	16.347	19.151	51.786	1.00 25.75	CPS5
ATOM	4317	CE2	PHE	74	14.750	17.896	53.092	1.00 26.75	CPS5
ATOM	4318	CZ	PHE	74	15.028	18.886	52.148	1.00 25.31	CPS5
ATOM	4319	С	PHE	74	20.260	15.241	53.674	1.00 23.42	CPS5
ATOM	4320	0	PHE	74	21.334	15.804	53.459	1.00 23.30	CPS5
ATOM	4321	N	GLN	75	20.141	14.207	54.504	1.00 24.48	CPS5
ATOM	4322	CA	GLN	75	21.284	13.688	55.245	1.00 24.75	CPS5
ATOM	4323	CB	GLN	75	20.804	12.774	56.382	1.00 24.94	CPS5
ATOM	4324	CG	GLN	75	20.012	13.515	57.455	1.00 24.64	CPS5
ATOM	4325	CD	GLN	75	20.838	14.550	58.200	1.00 24.25	CPS5
ATOM	4326	OE1	GLN	75	20.304	15.559	58.674	1.00 28.14	CPS5
ATOM	4327	NE2	GLN	75	22.141	14.308	58.319	1.00 22.66	CPS5
ATOM	4328	С	GLN	75	22.316	12.958	54.390	1.00 26.96	CPS5
ATOM	4329	0	GLN	75	23.423	12.684	54.861	1.00 27.29	CPS5
ATOM	4330	N	ASP	76	21.965	12.651	53.144	1.00 27.28	CPS5
ATOM	4331	CA	ASP	76	22.906	11.976	52.245	1.00 28.96	CPS5

FIG. 1A-75



SEP 0 9 2002

FIG. 1A-76

G. F1G.	ASS SUBCLASS	
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ATOM	4332	CB	ASP	76	22.171	11.187	51.157	1.00 28.71	CPS5
ATOM	4333	CG	ASP	76	21.422	10.002	51.695	1.00 30.19	CPS5
ATOM	4334	OD1	ASP	76	21.971	9.327	52.593	1.00 30.44	CPS5
ATOM	4335	OD2	2 ASP	76	20.296	9.733	51.211	1.00 30.21	CPS5
ATOM		C	ASP	76	23.787	13.007	51.552	1.00 29.00	
ATOM		ō	ASP	76	24.738	12.652	50.856		CPS5
ATOM		N	ILE	77	23.472	14.284		1.00 30.49	CPS5
ATOM		CA	ILE	77			51.743	1.00 28.00	CPS5
					24.207	15.354	51.080	1.00 27.42	CPS5
ATOM		CB	ILE	77	23.251	16.214	50.213	1.00 25.93	CPS5
ATOM		CG2		77	24.067	17.152	49.328	1.00 26.70	CPS5
ATOM			ILE	77	22.345	15.310	49.370	1.00 24.69	CPS5
ATOM			ILE	77	21.036	15.971	48.941	1.00 25.15	CPS5
ATOM		С	ILE	77	24.910	16.287	52.046	1.00 28.47	CPS5
ATOM	4345	0	ILE	77	24.287	16.853	52.943	1.00 29.75	CPS5
ATOM	4346	N	GLU	78	26.206	16.472	51.864	1.00 27.86	CPS5
ATOM	4347	CA	GLU	78	26.920	17.367	52.751	1.00 31.23	CPS5
ATOM	4348	CB	GLU	78	27.892	16.591	53.638	1.00 32.64	CPS5
ATOM	4349	CG	GLU	78	28.558	17.466	54.681	1.00 34.90	CPSS
ATOM	4350	CD	GLU	78	29.270	16.647	55.734	1.00 37.57	
ATOM	4351		GLU	78	30.334	16.072			CPS5
ATOM	4352	OE2		78			55.425	1.00 38.97	CPS5
ATOM	4353	C	GLU	78	28.753	16.568	56.866	1.00 38.56	CPS5
ATOM					27.676	18.468	52.042	1.00 31.73	CPS5
	4354	0	GLU	78	28.415	18.224	51.090	1.00 32.74	CPS5
ATOM	4355	N	ILE	79	27.481	19.691	52.508	1.00 32.96	CPS5
ATOM	4356	CA	ILE	79	28.177	20.821	51.932	1.00 35.99	CPS5
ATOM	4357	CB	ILE	79	27.265	22.044	51.818	1.00 36.51	CPS5
ATOM	4358	CG2	ILE	79	28.066	23.252	51.363	1.00 35.93	CPS5
ATOM	4359	CG1	ILE	79	26.129	21.738	50.842	1.00 37.54	CPS5
MOTA	4360	CD1	ILE	79	25.122	22.836	50.754	1.00 42.06	CPS5
ATOM	4361	С	ILE	79	29.342	21.145	52.842	1.00 38.38	CPS5
ATOM	4362	0	ILE	79	29.166	21.432	54.026	1.00 37.01	CPS5
ATOM	4363	N	ARG	80	30.543	21.075	52.290	1.00 42.32	
ATOM	4364	CA	ARG	80	31.729	21.371			CPS5
ATOM	4365	CB	ARG	80	32.690	20.180	53.070	1.00 46.50	CPS5
ATOM	4366	CG	ARG	80			53.091	1.00 46.70	CPS5
ATOM	4367	CD	ARG	80	32.116	18.913	53.670	1.00 48.52	CPS5
ATOM	4368	NE			33.151	17.798	53.687	1.00 49.02	CPS5
ATOM			ARG	80	32.519	16.508	53.945	1.00 50.86	CPS5
	4369	CZ	ARG	80	33.159	15.345	53.970	1.00 50.68	CPS5
ATOM	4370		ARG	80	34.465	15.303	53.757	1.00 50.94	CPS5
ATOM	4371		ARG	80	32.485	14.221	54.185	1.00 51.63	CPS5
ATOM	4372	С	ARG	80	32.444	22.545	52.459	1.00 48.41	CPS5
ATOM	4373	0	ARG	80	31.955	23.189	51.529	1.00 48.48	CPS5
ATOM	4374	N	LYS	81	33.616	22.820	53.003	1.00 51.83	CPS5
ATOM	4375	CA	LYS	81	34.448	23.892	52.507	1.00 54.26	CPS5
ATOM	4376	CB	LYS	81	34.388	25.099	53.445	1.00 55.70	CPS5
ATOM	4377	CG	LYS	81	32.994	25.704	53.578	1.00 58.10	CPS5
MOTA	4378	CD	LYS	81	33.014	26.958	54.439	1.00 59.69	CPS5
ATOM	4379	CE	LYS	81	31.606	27.467			
ATOM	4380	NZ	LYS	81	30.801		54.730	1.00 61.09	CPS5
ATOM	4381	c	LYS	81		26.502	55.540	1.00 61.28	CPS5
ATOM	4382	0	LYS	81	35.847	23.307	52.459	1.00 54.90	CPS5
ATOM	4383	N	ASP		36.305	22.695	53.427	1.00 54.56	CPS5
ATOM				82	36.504	23.452	51.314	1.00 55.76	CPS5
	4384	CA	ASP	82	37.855	22.940	51.151	1.00 56.67	CPS5
ATOM	4385	CB	ASP	82	38.281	23.026	49.683	1.00 56.75	CPS5
ATOM	4386	CG	ASP	82	37.874	24.337	49.031	1.00 56.88	CPS5
ATOM	4387		ASP	82	37.980	25.399	49.687	1.00 55.92	CPS5
ATOM	4388	OD2	ASP	82	37.457	24.301	47.853	1.00 57.36	CPS5



SEP 0 9 2002

FIG. 1A-77

G. FIG.	CLASS SUBCLASS		
APPROVED O.G. FIG.	(B)	DRAFTSMAN	

ATOM	4389	С	ASP	82	38.810	23.753	52.015	1.00 57.41	CPS5
ATOM	4390	0	ASP	82	38.377	24.523	52.874	1.00 56.93	CPS5
ATOM	4391	N	GLN	83	40.107	23.580	51.785	1.00 58.43	
ATOM	4392	CA	GLN	83	41.119	24.306	52.543	1.00 59.77	CPS5
ATOM	4393	CB	GLN	83	42.505	23.717	52.275		CPS5
ATOM	4394	CG	GLN	83	42.754	22.364	52.275	1.00 60.54	CPS5
ATOM	4395	CD	GLN	83				1.00 61.21	CPS5
ATOM	4396		GLN		42.737	22.424	54.432	1.00 61.78	CPS5
				83	41.674	22.447	55.054	1.00 62.24	CPS5
ATOM	4397	NE2		83	43.921	22.462	55.035	1.00 61.85	CPS5
ATOM	4398	C	GLN	83	41.117	25.793	52.189	1.00 60.23	CPS5
ATOM	4399	0	GLN		41.792	26.598	52.837	1.00 60.80	CPS5
ATOM	4400	N	ASN	84	40.359	26.153	51.157	1.00 59.89	CPS 5
ATOM	4401	CA	ASN	84	40.268	27.543	50.730	1.00 59.63	CPS5
MOTA	4402	CB	ASN	84	40.373	27.636	49.207	1.00 60.60	CPS5
MOTA	4403	CG	ASN	84	41.707	27.140	48.685	1.00 61.37	CPS5
ATOM	4404	OD1	ASN	84	42.761	27.667	49.044	1.00 61.62	CPS5
ATOM	4405	ND2	ASN	84	41.669	26.120	47.834	1.00 61.98	CPS5
ATOM	4406	С	ASN	84	38.956	28.160	51.199	1.00 59.10	
ATOM	4407	0	ASN	84	38.731	29.361	51.037	1.00 59.66	CPS5
ATOM	4408	N	GLY	85	38.095	27.330			CPS5
ATOM	4409	CA	GLY	85	36.818		51.780	1.00 57.75	CPS5
ATOM	4410	c	GLY	85	35.731	27.809	52.272	1.00 56.41	CPS5
ATOM	4411	Ö	GLY			27.794	51.213	1.00 55.75	CPS5
ATOM	4412	N		85	34.643	28.331	51.425	1.00 56.16	CPS5
			LYS	86	36.022	27.180	50.070	1.00 54.26	CPS5
MOTA MOTA	4413	CA	LYS	86	35.058	27.107	48.978	1.00 52.12	CPS5
	4414	CB	LYS	86	35.775	26.812	47.657	1.00 53.72	CPS5
ATOM	4415	CG	LYS	86	34.948	27.105	46.406	1.00 55.30	CPS5
ATOM	4416	CD	LYS	86	34.812	28.604	46.171	1.00 56.46	CPS5
ATOM	4417	CE	LYS	86	34.012	28.910	44.905	1.00 56.79	CPS5
ATOM	4418	NZ	LYS	86	32.619	28.397	45.007	1.00 57.01	CPS5
ATOM	4419	C	LYS	86	34.057	25.999	49.279	1.00 49.78	CPS5
ATOM	4420	0	LYS	86	34.420	24.944	49.806	1.00 49.58	CPS5
ATOM	4421	N	PRO	87	32.777	26.222	48.952	1.00 47.09	CPS5
ATOM	4422	CD	PRO	87	32.162	27.432	48.380	1.00 46.07	CPS5
ATOM	4423	CA	PRO	87	31.764	25.198	49.214	1.00 44.34	CPS5
ATOM	4424	CB	PRO	87	30.469	25.995	49.177	1.00 44.60	CPS5
ATOM	4425	CG	PRO	87	30.745	26.967	48.074	1.00 45.82	
ATOM	4426	С	PRO	87	31.776	24.098	48.158	1.00 40.83	CPS5
ATOM	4427	ō	PRO	87	31.837	24.382			CPS5
ATOM	4428	N	TYR	88	31.731	22.846	46.961	1.00 40.94	CPS5
ATOM	4429	CA	TYR	88	31.690		48.598	1.00 37.82	CPS5
ATOM	4430	CB	TYR	88		21.737	47.662	1.00 34.81	CPS5
ATOM	4431	CG	TYR	88	33.111	21.229	47.335	1.00 35.73	CPS5
ATOM	4432		TYR		33.795	20.385	48.390	1.00 34.31	CPS5
ATOM	4433		TYR	88	33.648	19.002	48.399	1.00 34.27	CPS5
ATOM	4434			88	34.303	18.212	49.339	1.00 34.82	CPS5
ATOM			TYR	88	34.615	20.966	49.354	1.00 35.40	CPS5
	4435		TYR	88	35.275	20.187	50.304	1.00 33.64	CPS5
ATOM	4436	CZ	TYR	88	35.112	18.812	50.290	1.00 35.08	CPS5
ATOM	4437	OH	TYR	88	35.730	18.028	51.239	1.00 35.18	CPS5
ATOM	4438	С	TYR	88	30.807	20.668	48.279	1.00 33.39	CPS5
ATOM	4439	0	TYR	88	30.627	20.633	49.497	1.00 32.83	CPS5
ATOM	4440	N	ILE	89	30.238	19.817	47.435	1.00 31.13	CPS5
MOTA	4441	CA	ILE	89	29.321	18.778	47.882	1.00 30.93	CPS5
ATOM	4442	CB	ILE	89	28.043	18.780	47.010	1.00 29.10	CPS5
ATOM	4443	CG2	ILE	89	27.189	17.547	47.303	1.00 27.98	CPS5
ATOM	4444	CG1		89	27.253	20.065	47.253	1.00 27.68	CPS5
ATOM	4445	CD1		89	26.041	20.215	46.364	1.00 27.88	CPS5
					20.041	20.215	40.304	1.00 27.97	CPSS



SEP 0 9 2002

FIG. 1A-78

F1G.	CLASS SUBCLASS	
0.0	CLASS	
APPROVED !	EY.	DRAFISHAN

ATOM	4446	С	ILE	89	29.873	17.362	47.863	1.00 32.51	CPS5
ATOM	4447	0	ILE	89	30.637	16.987	46.973	1.00 31.03	CPS5
ATOM	4448	N	ILE	90	29.462	16.582	48.858	1.00 33.80	CPS5
MOTA	4449	CA	ILE	90	29.837	15.180	48.960	1.00 35.56	CPS5
ATOM	4450	CB	ILE	90	30.776	14.928	50.144	1.00 37.43	CPS5
ATOM	4451	CG2	ILE	90	30.959	13.418	50.359	1.00 37.12	CPS5
MOTA	4452	CG1	ILE	90	32.116	15.608	49.875	1.00 38.91	CPS5
ATOM	4453	CD1	ILE	90	33.093	15.508	51.006	1.00 42.45	CPS5
ATOM	4454	C	ILE	90	28.564	14.363	49.156	1.00 36.47	CPS5
ATOM	4455	0	ILE	90	27.782	14.624	50.076	1.00 35.64	CPS5
ATOM	4456	N	CYS	91	28.348	13.400	48.269	1.00 36.91	CPS5
ATOM	4457	CA	CYS	91	27.189	12.520	48.340	1.00 40.22	CPS5
ATOM	4458	CB	CYS	91	26.132	12.945	47.328	1.00 37.91	CPS5
ATOM	4459	SG	CYS	91	24.623	11.970	47.401	1.00 39.23	CPS5
MOTA	4460	С	CYS	91	27.643	11.094	48.035	1.00 42.93	CPS5
ATOM	4461	0	CYS	91	27.983	10.771	46.895	1.00 42.83	CPS5
ATOM	4462	N	THR	92	27.648	10.245	49.056	1.00 46.74	CPS5
ATOM	4463	CA	THR	92	28.070	8.858	48.881	1.00 50.26	CPS5
ATOM	4464	CB	THR	92	28.080	8.106	50.238	1.00 51.61	CPS5
ATOM	4465		THR	92	28.496	6.748	50.035	1.00 52.93	CPS5
ATOM	4466	CG2	THR	92	26.693	8.130	50.876	1.00 52.67	CPS5
MOTA	4467	С	THR	92	27.175	8.110	47.890	1.00 51.62	CPS5
ATOM	4468	0	THR	92	27.656	7.285	47.108	1.00 51.98	CPS5
ATOM	4469	N	LYS	93	25.879	8.413	47.914	1.00 52.57	CPS5
ATOM	4470	CA	LYS	93	24.918	7.769	47.020	1.00 53.74	CPS5
ATOM	4471	CB	LYS	93	23.503	8.289	47.296	1.00 54.52	CPS5
ATOM	4472	CG	LYS	93	23.041	8.147	48.742	1.00 56.49	CPS5
ATOM	4473	CD	LYS	93	22.706	6.708	49.101	1.00 57.62	CPS5
ATOM	4474	CE	LYS	93	21.372	6.279	48.501	1.00 58.57	CPS5
ATOM	4475	NZ	LYS	93	20.218	7.009	49.109	1.00 59.31	CPS5
ATOM	4476	C	LYS	93	25.262	8.027	45.556	1.00 53.90	CPS5
MOTA	4477	0	LYS	93	24.681	7.419	44.656	1.00 54.01	CPS5
ATOM	4478	N	LEU	94	26.213	8.926	45.322	1.00 53.85	CPS5
ATOM	4479	CA	LEU	94	26.605	9.283	43.967	1.00 54.05	CPS5
ATOM	4480	CB	LEU	94	26.967	10.770	43.904	1.00 54.55	CPS5
ATOM	4481	CG	LEU	94	26.620	11.562	42.640	1.00 54.80	CPS5
MOTA	4482	CD1	LEU	94	27.225	12.951	42.751	1.00 54.69	CPS5
ATOM	4483	CD2	LEU	94	27.143	10.857	41.405	1.00 55.41	CPS5
ATOM	4484	С	LEU	94	27.780	8.466	43.452	1.00 54.05	CPS5
ATOM	4485	ō	LEU	94	28.797	8.322	44.130	1.00 54.64	CPS5
ATOM	4486	N	SER	95	27.626	7.934	42.246	1.00 53.47	CPS5
ATOM	4487	CA	SER	95	28.673	7.155	41.603	1.00 53.51	CPS5
ATOM	4488	CB	SER	95	28.131	6.559	40.299	1.00 54.31	CPS5
ATOM	4489	OG	SER	95	29.138	5.881	39.574	1.00 56.70	CPS5
MOTA	4490	C	SER	95	29.812	8.134	41.315	1.00 52.59	CPS5
MOTA	4491	ō	SER	95	29.589	9.345	41.279	1.00 53.14	CPS5
ATOM	4492	N	PRO	96	31.046	7.636	41.121	1.00 51.05	CPS5
ATOM	4493	CD	PRO	96	31.511	6.248	40.992	1.00 51.64	CPS5
ATOM	4494	CA	PRO	96	32.140	8.572	40.843	1.00 49.02	CPS5
ATOM	4495	СВ	PRO	96	33.252	7.670	40.285	1.00 50.01	CPS5
ATOM	4496	CG	PRO	96	32.537	6.387	39.898	1.00 51.26	CPS5
ATOM	4497	c	PRO	96	31.731	9.680	39.878	1.00 47.02	CPS5
ATOM	4498	ō	PRO	96	31.238	9.425	38.775	1.00 46.21	CPS5
ATOM	4499	N	ALA	97	31.931	10.917	40.313	1.00 44.30	CPS5
ATOM	4500	CA	ALA	97	31.566	12.063	39.499	1.00 41.77	CPS5
MOTA	4501	CB	ALA	97	30.055	12.176	39.425	1.00 40.64	CPS5
ATOM	4502	c	ALA	97	32.140	13.342	40.071	1.00 40.33	CPS5
		-		٠.	32.140	13.342	40.071	2.00 40.53	0.00



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SEP 0 9 2002

FIG. 1A-79

-16.	SUBCLASS	
0.G.F	CLASS	
AFFROVED	94	DRAFTSMA.H

MOTA	4503	0	ALA	97	32.593	13.382	41.216	1.00 40.58	CPS5
ATOM	4504	N	ALA	98	32.121	14.387	39.256	1.00 37.31	CPS5
MOTA	4505	CA	ALA	98	32.597	15.688	39.676	1.00 34.75	CPS 5
MOTA	4506	CB	ALA	98	33.398	16.340	38.561	1.00 35.64	CPS5
MOTA	4507	С	ALA	98	31.308	16.463	39.941	1.00 32.51	CPS5
ATOM	4508	0	ALA	98	30.407	16.478	39.107	1.00 31.77	CPS 5
ATOM	4509	N	VAL	99	31.204	17.061	41.119	1.00 29.38	CPS5
ATOM	4510	CA	VAL	99	30.017	17.823	41.476	1.00 26.77	CPS 5
ATOM	4511	CB	VAL	99	29.409	17.320	42.808	1.00 26.38	CPS 5
ATOM	4512	CG1	VAL	99	28.128	18.089	43.132	1.00 25.70	CPS5
ATOM	4513	CG2	VAL	99	29.110	15.821	42.708	1.00 26.03	CPS5
ATOM	4514	С	VAL	99	30.460	19.270	41.632	1.00 25.29	CPS5
ATOM	4515	0	VAL	99	31.518	19.541	42.192	1.00 24.54	CPS5
ATOM	4516	N	HIS	100	29.655	20.190	41.113	1.00 23.97	CPS5
ATOM	4517	CA	HIS	100	29.949	21.615	41.203	1.00 23.10	CPS5
ATOM	4518	CB	HIS	100	30.225	22.176	39.819	1.00 24.86	CPS5
ATOM	4519	CG	HIS	100	31.328	21.468	39.105	1.00 26.57	CPS5
ATOM	4520	CD2	HIS	100	31.297	20.480	38.181	1.00 27.57	CPS 5
ATOM	4521	ND1	HIS	100	32.660	21.719	39.358	1.00 28.54	CPS5
ATOM	4522	CE1	HIS	100	33.403	20.915	38.618	1.00 28.60	CPS5
ATOM	4523	NE2	HIS	100	32.599	20.155	37.894	1.00 28.27	CPS5
ATOM	4524	C	HIS	100	28.728	22.293	41.791	1.00 22.08	CPS5
ATOM	4525	0	HIS	100	27.602	21.917	41.475	1.00 21.49	CPS5
ATOM	4526	N	VAL	101	28.944	23.288	42.640	1.00 20.70	CPS5
ATOM	4527	CA	VAL	101	27.823	23.980	43.254	1.00 20.32	CPS5
ATOM	4528	CB	VAL	101	27.503	23.372	44.672	1.00 21.79	CPS5
ATOM	4529	CG1	VAL	101	28.687	23.560	45.614	1.00 21.73	CPS5
ATOM	4530	CG2	VAL	101	26.253	24.021	45.281	1.00 20.57	CPS5
ATOM	4531	С	VAL	101	28.137	25.462	43.385	1.00 20.62	CPS5
ATOM	4532	0	VAL	101	29.299	25.863	43.370	1.00 20.26	CPS5
ATOM	4533	N	SER	102	27.091	26.281	43.448	1.00 18.85	CPS5
ATOM	4534	CA	SER	102	27.256	27.709	43.670	1.00 18.73	CPS5
MOTA	4535	CB	SER	102	27.292	28.509	42.363	1.00 19.66	CPS5
ATOM	4536	OG	SER	102	27.474	29.886	42.685	1.00 19.70	CPS5
ATOM	4537	С	SER	102	26.037	28.118	44.489	1.00 19.25	CPS5
ATOM	4538	0	SER	102	24.931	27.684	44.200	1.00 17.98	CPS5
ATOM	4539	N	ILE	103	26.246	28.928	45.520	1.00 19.07	CPS5
ATOM	4540	CA	ILE	103	25.153	29.374	46.377	1.00 20.39	CPS5
ATOM	4541	CB	ILE	103	25.347	28.876	47.833	1.00 22.16	CPS5
ATOM	4542	CG2	ILE	103	24.216	29.404	48.736	1.00 22.36	CPS5
ATOM	4543	CG1	ILE	103	25.363	27.350	47.865	1.00 21.89	CPS5
ATOM	4544	CD1	ILE	103	25.821	26.762	49.214	1.00 24.06	CPS5
ATOM	4545	С	ILE	103	25.157	30.892	46.358	1.00 21.36	CPS5
ATOM	4546	0	ILE	103	26.225	31.512	46.304	1.00 21.80	CPS5
ATOM	4547	N	THR	104	23.968	31.489	46.374	1.00 21.34	CPS5
ATOM	4548	CA	THR	104	23.839	32.938	46.347	1.00 22.25	CPS5
ATOM	4549	CB	THR	104	23.591	33.450	44.901	1.00 24.00	CPS5
ATOM	4550	OG1	THR	104	23.661	34.887	44.864	1.00 24.60	CPS5
ATOM	4551	CG2	THR	104	22.235	32,998	44.399	1.00 23.88	CPS5
ATOM	4552	С	THR	104	22.705	33.376	47.276	1.00 23.21	CPS5
ATOM	4553	0	THR	104	21.831	32.579	47.641	1.00 21.95	CPS5
ATOM	4554	N	HIS	105	22.728	34.645	47.664	1.00 24.23	CPS5
ATOM	4555	CA	HIS	105	21.723	35.181	48.578	1.00 26.22	CPS5
ATOM	4556	CB	HIS	105	22.287	35.276	50.003	1.00 27.67	CPS5
ATOM	4557	CG	HIS	105	22.810	33.988	50.555	1.00 30.95	CPS5
ATOM	4558		HIS	105	24.036	33.417	50.475	1.00 32.56	CPS5
ATOM	4559		HIS	105	22.046	33.146	51.333	1.00 32.46	CPS5
							52.555		



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-80

ATOM 4560 CE1 HIS 105 22.777 1.00 32.44 32.114 51.713 CPS5 ATOM 4561 NE2 HIS 105 23.990 32.253 51.206 1.00 32.77 CPS5 ATOM 4562 C HIS 105 21,291 36.596 48.218 1.00 25.94 CPS5 ATOM 4563 0 HIS 105 22.037 37.344 47.584 1.00 25.81 ATOM 4564 N THR 106 20,077 36.944 48.630 1.00 25.98 ATOM 4565 CA THR 106 19.569 38.305 48.498 1.00 26.59 ATOM 4566 CB THR 106 18.474 38.498 47.436 1.00 26.91 ATOM 4567 OG1 THR 106 17.305 37.771 47.813 1.00 26.20 ATOM 4568 CG2 THR 106 18.963 38.070 46.062 1.00 25.16 ATOM 4569 С THR 106 18.946 38.516 49.870 1.00 27.65 ATOM 4570 0 THR 106 19.024 37.638 50.733 1.00 26.71 ATOM 4571 N LYS 107 18,330 39.667 50.086 1.00 28.18 ATOM 4572 CA LYS 107 17.716 39.938 51.377 1.00 29.86 ATOM 4573 CB LYS 107 17.103 41.345 51.366 1.00 32.21 CPS5 ATOM 4574 CG LYS 107 16.495 41.791 52.690 1.00 36.65 CPS5 ATOM 4575 CD LYS 107 15.848 52.540 43.171 1.00 40.32 CPS5 ATOM 4576 15.282 CE LYS 107 43.682 53.860 1.00 42.28 ATOM 4577 NZ. LYS 107 14.641 45.026 53.709 1.00 45.02 ATOM 4578 С LYS 107 16.645 38.910 51.754 1.00 29.02 CPS5 ATOM 4579 0 LYS 107 16.576 38.484 52,908 1.00 29.89 CPS5 ATOM 4580 N GLU 108 15.830 38.495 50.785 1.00 27.24 CPS 5 ATOM CA 4581 GLU 108 14.733 37.568 51.063 1.00 26.97 CPS 5 ATOM 4582 CB GLU 108 13.428 38.156 50.525 1.00 29.17 CPS 5 ATOM 4583 CG GLU 108 13.129 39.552 51.030 1.00 35.90 CPS 5 ATOM 4584 CD GLU 108 11.758 40.043 50.612 1.00 40.16 CPS5 ATOM 4585 OE1 GLU 108 11.459 40.044 49.397 1.00 43.68 CPS5 ATOM 4586 OE2 GLU 108 10.975 40.436 51.505 1.00 44.69 CPS5 ATOM 4587 С GLU 108 14.855 36.149 50.527 1.00 24.76 CPS5 ATOM 4588 0 GLU 108 14.007 35.300 50.823 1.00 23.74 CPS 5 ATOM 4589 N TYR 109 15.889 35.888 49.738 1.00 23.62 CPS 5 ATOM 4590 CA TYR 109 16.045 34.564 49.137 1.00 23.16 CPS 5 ATOM 4591 CB TYR 109 15.695 34.627 47.645 1.00 23.09 CPS5 ATOM 4592 CG TYR 109 14.286 35.052 47.352 1.00 23.49 CPS5 ATOM 4593 CD1 TYR 109 13.243 34.135 47.403 1.00 24.28 CPS5 ATOM 4594 CE1 TYR 109 11.931 34.529 47.199 1.00 24.85 CPSS ATOM 4595 CD2 TYR 109 13.982 36.390 47.080 1.00 26.20 CDSS ATOM 4596 CE2 TYR 109 12.667 36.797 46.874 1.00 25.83 CPS5 ATOM 4597 CZTYR 109 11.648 35.861 46.937 1.00 25.55 CPS 5 ATOM 4598 OH TYR 109 10.341 36.243 46.769 1.00 26.59 CPS 5 ATOM 4599 c TYR 109 17.438 33.976 49.230 1.00 22.83 CPS5 ATOM 4600 0 TYR 109 18.421 34.691 49.403 1.00 23.71 CPS5 ATOM 4601 N ALA 110 17.490 32.650 49.128 1.00 21.41 CPS5 ATOM 4602 CA ALA 110 18.744 31.912 49.055 1.00 21.16 CPS5 ATOM 4603 CB ALA 110 18.924 30.988 50.258 1.00 20.41 CPS5 ATOM 4604 С ALA 110 18.536 31.089 47.785 1.00 20.71 CPS5 ATOM 4605 O ALA 110 17.415 1.00 21.39 30.635 47.508 CPS5 ATOM 4606 M ALA 111 19.589 30.915 46.991 1.00 19.32 CPS5 ATOM 4607 מי ALA 111 19.467 30.131 45.771 1.00 18.05 CPS5 ATOM 4608 CB ALA 111 19.215 31.033 44.575 1.00 18.98 CPS5 ATOM 4609 С ALA 111 20.734 29.344 45.550 1.00 19.39 CPS5 ATOM 4610 ALA 0 111 21.800 29.707 46.050 1.00 18.83 CPS5 ATOM 4611 N ALA 112 20.623 28.269 44.786 1.00 18.45 CPS5 ATOM 4612 CA ALA 112 21.784 27,451 44.508 1.00 19.52 CPS5 ATOM 4613 CB ALA 112 22.008 26.481 45.655 1.00 19.65 CPS5 ATOM 4614 С

26.679

26.442

26.311

43.212

42.764

1.00 18.81

1.00 17.20

42.599 1.00 19.37

CPSS

CPS5

CPS5

21.617

20.502

22.733

ALA 112

GLN 113

ATOM

ATOM

4615 0 ALA 112

4616 N

SUBCLASS <u>.</u> 10 CLASS 0



SEP 0 9 2002

FIG. 1A-81

TECH CENTER 1600/2900

ATOM	4617	CA	GLN	113	22.663	25.499	41.400	1.00 20.01	CPS5
ATOM	4618	CB	GLN		22.890	26.321	40.135	1.00 23.47	CPS5
ATOM	4619	CG	GLN	113	24.249	26.942	40.040	1.00 26.43	CPS5
ATOM	4620	CD	GLN	113	24.463	27.640	38.705	1.00 30.41	CPS 5
ATOM	4621		GLN	113	25.506	28.234	38.467	1.00 29.83	CPS5
ATOM	4622		GLN	113	23.466	27.567	37.831	1.00 33.75	CPS5
ATOM	4623	C	GLN	113	23.735	24.439	41.518	1.00 19.96	CPS 5
ATOM	4624	0	GLN	113	24.753	24.633	42.177	1.00 19.44	CPS5
ATOM	4625	N	VAL	114	23.504	23.312	40.869	1.00 19.35	CPS5
ATOM	4626	CA	VAL	114	24.462	22.221	40.924	1.00 19.11	CPS5
ATOM	4627	CB	VAL	114	23.960	21.111	41.897	1.00 18.72	CPS 5
ATOM	4628		VAL	114	24.791	19.828	41.721	1.00 20.30	CPS5
ATOM	4629		VAL	114	24.043	21.603	43.344	1.00 20.16	CPS5
ATOM	4630	С	VAL	114	24.589	21.611	39.538	1.00 19.40	CPS5
ATOM	4631	0	VAL	114	23.618	21.590	38.781	1.00 19.86	CPS5
ATOM	4632	N	VAL	115	25.792	21.159	39.201	1.00 19.59	CPS5
ATOM	4633	CA	VAL	115	26.017	20.436	37.956	1.00 19.26	CPS5
ATOM	4634	CB	VAL	115	26.879	21.202	36.928	1.00 20.70	CPS5
ATOM	4635		VAL	115	27.182	20.280	35.725	1.00 19.97	CPS5
ATOM	4636		VAL	115	26.131	22.443	36.433	1.00 19.15	CPS5
ATOM	4637	С	VAL	115	26.780	19.172	38.359	1.00 22.16	CPS5
ATOM	4638	0	VAL	115	27.765	19.248	39.092	1.00 21.19	CPS5
ATOM	4639	N	ILE	116	26.291	18.018	37.920	1.00 23.19	CPS 5
ATOM	4640	CA	ILE	116	26.965	16.749	38.201	1.00 25.23	CPS5
ATOM	4641	CB	ILE	116	25.983	15.681	38.761	1.00 24.21	CPS5
ATOM	4642		ILE	116	26.717	14.347	38.952	1.00 24.03	CPS5
ATOM	4643		ILE	116	25.401	16.139	40.106	1.00 24.21	CPS5
ATOM	4644		ILE	116	24.294	15.209	40.635	1.00 22.70	CPS5
ATOM	4645	С	ILE	116	27.521	16.243	36.866	1.00 26.72	CPS5
ATOM	4646	0	ILE	116	26.788	16.165	35.881	1.00 25.85	CPS5
ATOM	4647	N	GLU	117	28.809	15.914	36.835	1.00 30.40	CPS5
ATOM	4648	CA	GLU	117	29.447	15.401	35.615	1.00 35.53	CPS5
ATOM ATOM	4649	CB	GLU	117	30.792	16.064	35.352	1.00 36.89	CPS5
ATOM	4650	CG	GLU	117	30.816	17.554	35.274	1.00 39.07	CPS5
ATOM	4651	CD	GLU	117	32.168	18.036	34.808	1.00 39.75	CPS5
ATOM	4652		GLU	117	32.457	17.877	33.605	1.00 40.89	CPS5
ATOM	4653 4654		GLU	117	32.948	18.547	35.641	1.00 40.65	CPS5
ATOM	4655	C	GLU	117	29.735	13.915	35.771	1.00 38.76	CPS5
ATOM	4656	O N	GLU ALA	117	30.317	13.501	36.782	1.00 38.92	CPS5
ATOM	4657	CA	ALA	118	29.364	13.131	34.761	1.00 41.50	CPS5
ATOM	4658	CB	ALA	118	29.596	11.689	34.784	1.00 44.75	CPS5
ATOM	4659	C	ALA	118	29.047	11.049	33.508	1.00 45.12	CPS5
ATOM	4660	OT1		118 118	31.095	11.422	34.899	1.00 46.14	CPS5
ATOM	4661		ALA	118	31.885	12.266	34.413	1.00 46.30	CPS5
ATOM	4662	C	GLY	118	31.460	10.367	35.466	1.00 48.44	CPS5
ATOM	4663	ō	GLY	1	34.929	20.508	32.382	1.00 33.16	CPS6
ATOM	4664	N	GLY	1	35.455	21.500	31.885	1.00 34.15	CPS6
ATOM	4665	CA	GLY	1	36.363	18.424	32.401	1.00 38.41	CPS6
ATOM	4666	N	ILE	2	35.171	19.118	31.815	1.00 34.91	CPS6
ATOM	4667	CA	ILE	2	34.133	20.587	33.435	1.00 30.97	CPS6
ATOM	4668	CB	ILE	2	33.824	21.875	34.039	1.00 28.64	CPS6
ATOM	4669	CG2	ILE	2	32.405	21.855	34.627	1.00 27.89	CPS6
ATOM	4670		ILE	2	32.168	23.101	35.474	1.00 27.12	CPS6
ATOM	4671		ILE	2	31.386	21.726	33.490	1.00 28.03	CPS6
ATOM	4672	C	ILE	2	29.965	21.432	33.954	1.00 28.46	CPS6
ATOM	4673	ō	ILE	2	34.810	22.262	35.134	1.00 28.03	CPS6
		-		-	35.117	21.463	36.011	1.00 27.12	CPS6



SUBCLASS

20

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SEP 0 9 2002

FIG. 1A-82

TECH CENTER 1600/2900

ATOM 4674 23.492 N TYR 3 35.305 35.080 1.00 26.59 CPS6 ATOM 4675 CA TYR 3 36.234 23.970 36.101 1.00 26.25 CPS6 ATOM 4676 CB TYR 3 37.102 25.091 35.540 1.00 27.53 CPS6 ATOM 4677 CG TYR 3 38.027 25.703 36.570 1.00 31.25 CPS ATOM 4678 CD1 TYR 3 39.171 25.027 36.999 1.00 32.43 CPS6 ATOM 4679 CE1 TYR 3 40.006 25.568 37.978 1.00 35.68 CPS6 ATOM 4680 CD2 TYR 3 37.738 26.937 37.146 1.00 31.55 CPS6 ATOM 4681 CE2 27.489 TYR 3 38.563 38.126 1.00 35.40 CPS6 ATOM 4682 czTYR 2 39.697 26.800 38.537 1.00 36.39 CPS6 ATOM 4683 ОН TYR 3 40.525 27.355 1.00 39.51 39.488 CPS6 ATOM 4684 C TYR 3 35.451 24.482 37.316 1.00 25.81 CPS6 ATOM 4685 0 TVD 3 35.762 24.145 38.469 1.00 24.16 CPS6 ATOM 4686 N GT.Y 4 34.437 25.301 37.058 1.00 22.42 CPS6 ATOM 4687 CA GLY 4 33.630 25.823 38.147 1.00 22.32 CPS ATOM 4688 С GLY 4 32.365 26.494 37.642 1.00 20.34 CPS6 ATOM 4689 O GLY. 4 32.280 26.799 36.461 1.00 19.69 CPSE ATOM 4690 N TLE 5 31.389 26.704 38.525 1.00 20.01 CDSE ATOM 4691 CA ILE 5 30.140 27.366 38,143 1.00 20.35 CPS6 ATOM 4692 CB TLE 5 28.947 26.382 38.097 1.00 20.14 CPSE ATOM 4693 CG₂ ILE 5 29.291 25.224 37.159 1.00 19.26 CPS6 ATOM 4694 CGI ILE 5 28.600 25.876 39.507 1.00 19.61 CPSE ATOM 4695 CD1 ILE 5 27.418 24.871 39.535 1.00 21.63 CPS ATOM 4696 c ILE 5 29.832 28.481 39.119 1.00 20.43 CRSE ATOM 4697 TI.E 5 30.337 28.505 40.242 1.00 20.18 CPSE ATOM 4698 N GLY 6 29.009 29.426 38.686 1.00 19.58 CDCC ATOM 4699 CA GLY 6 28.681 30.532 39.560 1.00 19.69 CPSE ATOM 4700 c GLY 6 27.279 31.023 39.287 1.00 19.25 CPSE ATOM 4701 0 GLY 6 26.842 31.080 38.135 1.00 17.69 CDSC ATOM 4702 N LEU 7 26.581 31.374 40.358 1.00 19.31 CPS6 ATOM 4703 CA LEU 7 25.214 31.865 1.00 20.65 40.262 CPS6 ATOM 4704 CB LEU 7 24.249 30.808 40.811 1.00 20.48 CPS6 ATOM 4705 CG LEU 7 22.781 31.222 40.967 1.00 21.08 CPSE ATOM 4706 CD1 LEU 7 22.175 31.455 39.576 1.00 22.40 CPS6 ATOM 4707 CD2 LEU 7 22.017 30.132 41.724 1.00 21.05 CPS6 ATOM 4708 С LEU 7 25.108 33.114 41.116 1.00 20.36 CPS6 ATOM 4709 0 LEU 7 25.687 33.180 42.193 1.00 21.58 CPS6 ATOM 4710 N ASP 8 24.387 34.114 40.631 1.00 20.16 CPS6 ATOM 4711 CA ASP 8 24.188 35.310 41.423 1.00 21.86 CPS6 ATOM 4712 CB ASP 8 25.261 36.368 41.151 1.00 23.79 CPS6 ATOM 4713 CĠ ASP я 25.018 37.637 41.948 1.00 26.23 CPS6 ATOM 4714 OD1 ASP 8 24.287 38.523 41.462 1.00 26.66 CPS6 ATOM 4715 OD2 ASP 8 25.523 37.725 43.081 1.00 27.19 CPS6 ATOM 4716 С ASP я 22.838 35.935 41.173 1.00 21.30 CPS6 ATOM 4717 0 ASP 8 22.379 35.977 40.041 1.00 20.01 CPS6 ATOM 4718 N ILE 9 22.184 36.384 42.242 1.00 20.98 CPS6 ATOM 4719 CA ILE 9 20.911 37.081 42.099 1.00 20.91 CPS6 ATOM 4720 CB ILE 9 19.733 36.347 42.787 1.00 21.99 CPS6 ATOM 4721 CG2 ILE 9 18.456 37.172 42.639 1.00 20.05 CPS6 ATOM 4722 CG1 ILE 9 19.543 34.963 42.159 1.00 20.50 CPS6 ATOM 4723 CD1 ILE 9 18.405 34.165 42.754 1.00 21.55 CPS6 ATOM 4724 С ILE 9 21.160 38.402 42.803 1.00 22.15 CPS6 ATOM 4725 0 TLE 9 21.683 38.420 43.918 1.00 23.20 CPS6 ATOM 4726 N THR 10 20.813 39.505 42.148 1 00 24 06 CPS6 ATOM 4727 CA THR 10 21.033 40.826 42.722 1.00 25.03 CPS6 ATOM 4728 CB THR 10 22.125 41.578 41.915 1.00 27.35 CPS6 ATOM 4729 OG1 THR 10 23.375 40.882 42.054 1.00 27.27 CPS6 ATOM 4730 CG2 THR 10 22.299 43.006

42.413

1.00 28.83

CPS6



SEP 0 9 2002

FIG. 1A-83

.16.	SUBCLASS		
0.6.	CLASS		
APPROVES	λs	DRAFTSKAM	

ATOM	4731	C	THR	10	19.734	41.626	42.734	1.00 25.30	CPS6
ATOM	4732	0	THR	10	18.978	41.620	41.762	1.00 24.09	CPS6
ATOM	4733	N	GLU	11	19.475	42.290	43.857	1.00 24.60	CPS6
ATOM	4734	CA	GLU	11	18.278	43.112	44.025	1.00 25.85	CPS6
ATOM	4735	CB	GLU	11	18.012	43.306	45.525	1.00 26.85	CPS6
ATOM	4736	CG	GLU	11	16.635	43.843	45.872	1.00 30.57	CPS6
ATOM	4737	CD	GLU	11	16.506	44.224	47.342	1.00 33.54	CPS6
ATOM	4738		GLU	11	17.435	43.928	48.136	1.00 34.46	
ATOM	4739	0E2		11	15.469	44.821	47.701		CPS6
ATOM	4740	C	GLU	11	18.533	44.467		1.00 34.21	CPS6
ATOM	4741	ō	GLU	11	19.499		43.354	1.00 25.21	CPS6
ATOM	4742	N	LEU	12	17.687	45.150	43.694	1.00 26.16	CPS6
ATOM	4743	CA	LEU			44.855	42.402	1.00 26.01	CPS6
				12	17.870	46.138	41.713	1.00 28.08	CPS6
ATOM	4744	CB	LEU	12	16.733	46.381	40.707	1.00 28.52	CPS6
ATOM	4745	CG	LEU	12	16.880	45.889	39.264	1.00 31.49	CPS6
ATOM	4746		LEU	12	17.467	44.495	39.234	1.00 30.71	CPS6
ATOM	4747		LEU	12	15.530	45.921	38.573	1.00 32.17	CPS6
ATOM	4748	С	LEU	12	17.926	47.301	42.708	1.00 29.26	CPS6
ATOM	4749	0	LEU	12	18.732	48.223	42.553	1.00 29.98	CPS6
MOTA	4750	N	ALA	13	17.067	47.258	43.725	1.00 29.78	CPS6
ATOM	4751	CA	ALA	13	17.027	48.315	44.733	1.00 30.29	CPS6
ATOM	4752	CB	ALA	13	15.901	48.042	45.741	1.00 31.01	CPS6
ATOM	4753	С	ALA	13	18.364	48.447	45.460	1.00 31.44	CPS6
ATOM	4754	0	ALA	13	18.774	49.551	45.825	1.00 31.56	CPS6
ATOM	4755	N	ARG	14	19.048	47.327	45.669	1.00 32.19	CPS6
ATOM	4756	CA	ARG	14	20.338	47.357	46.352	1.00 32.19	
ATOM	4757	CB	ARG	14	20.745	45.940	46.768		CPS6
ATOM	4758	CG	ARG	14				1.00 35.66	CPS6
ATOM	4759	CD	ARG	14	22.097 22.314	45.852	47.437	1.00 39.95	CPS6
ATOM	4760	NE	ARG			44.493	48.078	1.00 42.90	CPS6
ATOM	4761	CZ		14	23.727	44.261	48.363	1.00 46.95	CPS6
ATOM			ARG	14	24.577	43.675	47.524	1.00 48.91	CPS6
	4762		ARG	14	24.163	43.247	46.338	1.00 50.22	CPS6
ATOM	4763		ARG	14	25.850	43.523	47.868	1.00 50.46	CPS6
ATOM	4764	С	ARG	14	21.415	48.002	45.469	1.00 32.36	CPS6
ATOM	4765	0	ARG	14	22.268	48.747	45.961	1.00 31.82	CPS6
ATOM	4766	N	ILE	15	21.381	47.719	44.171	1.00 31.44	CPS6
ATOM	4767	CA	ILE	15	22.337	48.326	43.247	1.00 31.99	CPS6
ATOM	4768	CB	ILE	15	22.153	47.777	41.817	1.00 32.07	CPS6
ATOM	4769	CG2		15	22.911	48.638	40.813	1.00 31.65	CPS6
ATOM	4770	CG1	ILE	15	22.655	46.333	41.752	1.00 32.16	CPS6
ATOM	4771	CD1	ILE	15	24.156	46.184	42.013	1.00 33.75	CPS6
ATOM	4772	C	ILE	15	22.113	49.843	43.236	1.00 32.92	CPS6
ATOM	4773	0	ILE	15	23.062	50.627	43.265	1.00 32.09	CPS6
ATOM	4774	N	ALA	16	20.851	50.254	43.201	1.00 33.77	CPS6
ATOM	4775	CA	ALA	16	20.520	51.677	43.194	1.00 36.34	CPS6
ATOM	4776	CB	ALA	16	19.014	51.860	43.063	1.00 36.06	CPS6
ATOM	4777	С	ALA	16	21.030	52.356	44.467	1.00 38.13	CPS6
ATOM	4778	0	ALA	16	21.491	53.498	44.427	1.00 38.48	CPS6
ATOM	4779	N	SER	17	20.951	51.648	45.590	1.00 40.20	CPS6
ATOM	4780	CA	SER	17	21.415	52.175	46.871	1.00 43.01	
ATOM	4781	CB	SER	17	20.959	51.268			CPS6
ATOM	4782	OG	SER	17	19.549		48.017	1.00 43.08	CPS6
ATOM	4783	C	SER	17		51.302	48.157	1.00 45.35	CPS6
ATOM	4784	0	SER	17	22.934	52.320	46.919	1.00 44.34	CPS6
ATOM	4785	N	MET		23.456	53.311	47.432	1.00 44.28	CPS6
ATOM	4786	CA	MET	18	23.644	51.323	46.402	1.00 45.43	CPS6
ATOM	4787	CB	MET	18	25.100	51.370	46.390	1.00 47.02	CPS6
ATOM	4/0/	CB	MET	18	25.678	50.035	45.917	1.00 48.11	CPS6

SEP 0 9 2002

FIG. 1A-84

TECH CENTER 1600/2900

APPROVED 0.G. F1G.
BY CLASS SUBCLASS
ORAFISHAM

ATOM	4788	CG	MET	18	25.502	48.901	46.906	1.00 49.87	CPS6
ATOM	4789	SD	MET	18	26.307	47.401	46.338	1.00 54.02	CPS6
ATOM	4790	CE	MET	18	24.997	46.663	45.390	1.00 52.20	CPS6
ATOM	4791	С	MET	18	25.586	52.485	45.475	1.00 47.28	CPS6
ATOM	4792	0	MET	18	26.533	53.196	45.799	1.00 47.27	CPS6
MOTA	4793	14	ALA	19	24.923	52.636	44.334	1.00 47.28	CPS6
MOTA	4794	CA	ALA	19	25.284	53.658	43.361	1.00 48.35	CPS6
ATOM	4795	CB	ALA	19	24.558	53.397	42.049	1.00 47.94	CPS6
ATOM	4796	С	ALA	19	24.956	55.059	43.867	1.00 49.67	CPS6
ATOM	4797	0	ALA	19	25.644	56.031	43.539	1.00 48.84	CPS6
ATOM	4798	N	GLY	20	23.895	55.159	44.659	1.00 50.28	CPS6
ATOM	4799	CA	GLY	20	23.501	56.448	45.188	1.00 52.81	CPS6
ATOM	4800	C	GLY	20	24.379	56.884	46.342	1.00 53.84	CPS6
ATOM	4801	0	GLY	20	24.504	58.077	46.612	1.00 54.96	CPS6
ATOM	4802	N	ARG	21	24.996	55.919	47.017	1.00 54.88	CPS6
ATOM ATOM	4803 4804	CA	ARG	21	25.853	56.215	48.157	1.00 56.13	CPS6
ATOM	4804	CB	ARG	21	25.694	55.134	49.228	1.00 57.83	CPS6
ATOM	4805	CD	ARG ARG	21 21	24.308	55.086	49.857	1.00 60.18	CPS6
ATOM	4807	NE	ARG	21	24.275	54.226	51.123	1.00 62.40	CPS6
ATOM	4808	CZ	ARG	21	24.085 25.003	52.797	50.866	1.00 64.82	CPS6
ATOM	4809		ARG	21	26.207	51.979 52.434	50.352	1.00 65.81	CPS6
ATOM	4810	NH2		21	24.714	50.695	50.024 50.175	1.00 66.03	CPS6
ATOM	4811	C	ARG	21	27.327	56.359	47.802	1.00 65.70	CPS6
ATOM	4812	ō	ARG	21	28.113	56.882	48.591	1.00 56.17 1.00 56.98	CPS6
ATOM	4813	N	GLN	22	27.710	55.896	46.619	1.00 56.98 1.00 55.40	CPS6 CPS6
ATOM	4814	CA	GLN	22	29.104	55.992	46.207	1.00 54.24	CPS6
ATOM	4815	СВ	GLN	22	29.637	54.619	45.795	1.00 55.16	CPS6
ATOM	4816	CG	GLN	22	29.456	53.533	46.836	1.00 57.52	CPS6
ATOM	4817	CD	GLN	22	30.179	52.251	46.467	1.00 58.37	CPS6
ATOM	4818	OE1	GLN	22	30.060	51.236	47.154	1.00 59.62	CPS6
ATOM	4819	NE2	GLN	22	30.940	52.294	45.378	1.00 59.05	CPS6
MOTA	4820	С	GLN	22	29.281	56.953	45.044	1.00 52.16	CPS6
ATOM	4821	0	GLN	22	28.312	57.363	44.402	1.00 51.84	CPS6
ATOM	4822	N	LYS	23	30.531	57.325	44.793	1.00 49.79	CPS6
ATOM	4823	CA	LYS	23	30.848	58.203	43.679	1.00 47.03	CPS6
ATOM	4824	CB	LYS	23	31.906	59.240	44.078	1.00 48.67	CPS6
ATOM	4825	CG	LYS	23	32.117	60.319	43.025	1.00 50.00	CPS6
ATOM	4826	CD	LYS	23	33.404	61.106	43.232	1.00 51.39	CPS6
ATOM	4827	CE	LYS	23	33.384	61.925	44.506	1.00 52.42	CPS6
ATOM	4828	NZ	LYS	23	34.570	62.835	44.558	1.00 53.74	CPS6
ATOM	4829	C	LYS	23	31.406	57.280	42.595	1.00 43.64	CPS6
ATOM ATOM	4830	0	LYS	23	32.259	56.433	42.866	1.00 43.39	CPS6
ATOM	4831 4832	N	ARG	24	30.898	57.421	41.379	1.00 40.62	CPS6
ATOM		CA	ARG	24	31.363	56.603	40.266	1.00 38.09	CPS6
ATOM	4833 4834	CB	ARG	24	32.806	56.991	39.919	1.00 38.24	CPS6
ATOM	4834	CD	ARG ARG	24	32.935	58.400	39.340	1.00 38.55	CPS6
ATOM	4836	NE	ARG	24	34.348	58.672	38.853	1.00 38.30	CPS6
ATOM	4837	CZ	ARG	24	35.297	58.859	39.948	1.00 39.05	CPS6
ATOM	4838		ARG	24 24	35.511	60.019	40.561	1.00 39.71	CPS6
ATOM	4839		ARG	24	34.846	61.108	40.190	1.00 39.61	CPS6
ATOM	4840	C	ARG	24	36.396	60.092	41.543	1.00 39.47	CPS6
ATOM	4841	ō	ARG	24	31.266 32.202	55.086	40.500	1.00 35.99	CPS6
ATOM	4842	N	PHE	25	32.202	54.339	40.206	1.00 34.55	CPS6
ATOM	4843	CA	PHE	25	29.959	54.627 53.196	41.026	1.00 33.55	CPS6
ATOM	4844	CB	PHE	25	28.647	52.938	41.251	1.00 31.77	CPS6
					20.04/	32.936	42.012	1.00 32.24	CPS6



SEP 0 9 2002 **TECH CENTER 1600/2900**

FIG. 1A-85

CLASS |SUBCLASS

ATOM	4845	CG	PHE	25	28.331	51.481	42.211	1.00 31.39	CPS6
ATOM	4846	CD1	PHE	25	27.306	50.879	41.495	1.00 33.76	CPS6
ATOM	4847	CD2	PHE	25	29.069	50.709	43.102	1.00 32.67	CPS6
ATOM	4848	CE1	PHE	25	27.021	49.524	41.663	1.00 32.84	CPS6
ATOM	4849	CE2		25	28.794	49.354	43.277	1.00 32.53	CPS6
ATOM	4850	CZ	PHE	25	27.764	48.763	42.553	1.00 32.75	CPS6
ATOM	4851	c	PHE	25	29.943	52.489	39.887	1.00 30.17	CPS6
ATOM	4852	ō	PHE	25	30.573	51.446	39.706	1.00 28.44	CPS6
ATOM	4853	N	ALA	26	29.236	53.074	38.923	1.00 29.20	CPS6
ATOM	4854	CA	ALA	26	29.158	52.484	37.592	1.00 28.94	CPS6
ATOM	4855	CB	ALA	26	28.244	53.319	36.697	1.00 29.36	CPS6
ATOM	4856	c	ALA	26	30.540	52.376	36.961	1.00 28.91	CPS6
ATOM	4857	ō	ALA	26	30.857	51.378	36.325	1.00 26.93	CPS6
ATOM	4858	N	GLU	27	31.358	53.411	37.144	1.00 28.69	CPS6
ATOM	4859	CA	GLU	27	32.701	53.434	36.576	1.00 29.76	CPS6
ATOM	4860	CB	GLU	27	33.317	54.829	36.730	1.00 30.26	CPS6
ATOM	4861	CG	GLU	27	32.737	55.916	35.822	1.00 32.04	CPS6
ATOM	4862	CD	GLU	27	31.325	56.344	36.195	1.00 32.04	CPS6
ATOM	4863		GLU	27	30.902	56.135	37.353	1.00 32.41	CPS6
ATOM	4864		GLU	27	30.502	56.914	35.318	1.00 32.41	CPS6
			GLU	27	33.622	52.399	37.224	1.00 37.48	CPS6
ATOM	4865	C		27			36.673	1.00 29.53	CPS6
ATOM	4866	0	GLU		34.661	52.040			
ATOM	4867	N	ARG	28	33.243	51.927	38.402	1.00 30.48	CPS6
MOTA	4868	CA	ARG	28	34.040	50.934	39.107	1.00 32.10	CPS6
ATOM	4869	CB	ARG	28	33.782	51.051	40.611	1.00 35.59	CPS6
ATOM	4870	CG	ARG	28	34.480	50.013	41.467	1.00 40.15	CPS6
ATOM	4871	CD	ARG	28	34.042	50.172	42.911	1.00 44.70	CPS6
MOTA	4872	NE	ARG	28	33.719	48.891	43.529	1.00 48.06	CPS6
ATOM	4873	CZ	ARG	28	33.004	48.764	44.642	1.00 50.43	CPS6
ATOM	4874		ARG	28	32.535	49.845	45.258	1.00 51.09	CPS6
ATOM	4875		ARG	28	32.755	47.558	45.139	1.00 51.52	CPS6
ATOM	4876	С	ARG	28	33.677	49.526	38.621	1.00 30.71	CPS6
ATOM	4877	0	ARG	28	34.546	48.659	38.464	1.00 32.13	CPS6
ATOM	4878	N	ILE	29	32.391	49.316	38.364	1.00 28.03	CPS6
ATOM	4879	CA	ILE	29	31.891	48.016	37.922	1.00 26.37	CPS6
MOTA	4880	CB	ILE	29	30.387	47.854	38.270	1.00 25.85	CPS6
ATOM	4881	CG2		29	29.886	46.496	37.802	1.00 25.90	CPS6
ATOM	4882	CG1		29	30.164	48.051	39.776	1.00 27.54	CPS6
ATOM	4883		ILE	29	30.962	47.113	40.667	1.00 27.66	CPS6
ATOM	4884	С	ILE	29	32.030	47.746	36.421	1.00 25.65	CPS6
ATOM	4885	0	ILE	29	32.327	46.617	36.017	1.00 24.93	CPS6
ATOM	4886	N	LEU	30	31.820	48.784	35.609	1.00 23.77	CPS6
ATOM	4887	CA	LEU	30	31.844	48.651	34.158	1.00 24.32	CPS6
ATOM	4888	CB	LEU	30	30.665	49.429	33.567	1.00 24.16	CPS6
ATOM	4889	CG	LEU	30	29.282	49.141	34.169	1.00 25.20	CPS6
ATOM	4890		LEU	30	28.251	50.068	33.540	1.00 24.33	CPS6
ATOM	4891	CD2	LEU	30	28.898	47.695	33.927	1.00 23.57	CPS6
ATOM	4892	С	LEU	30	33.121	49.071	33.433	1.00 24.24	CPS6
MOTA	4893	0	LEU	30	33.820	49.996	33.845	1.00 23.43	CPS6
ATOM	4894	N	THR	31	33.404	48.376	32.341	1.00 23.91	CPS6
MOTA	4895	CA	THR	31	34.573	48.676	31.523	1.00 25.21	CPS6
ATOM	4896	CB	THR	31	34.999	47.461	30.695	1.00 25.51	CPS6
ATOM	4897	OG1	THR	31	33.972	47.150	29.739	1.00 24.34	CPS6
ATOM	4898	CG2	THR	31	35.245	46.265	31.597	1.00 24.28	CPS6
MOTA	4899	С	THR	31	34.219	49.798	30.553	1.00 26.00	CPS6
ATOM	4900	0	THR	31	33.071	50.247	30.490	1.00 25.37	CPS
ATOM	4901	N	ARG	32	35.202	50.240	29.782	1.00 27.55	CPS



SEP 0 9 2002

TECH CENTER 1600/8900

9.0.G. F1G.	CLASS SUBCLASS	2
APPROVEC	θХ	DRAF ISM.

ATOM	4902	CA	ARG	32	34.976	51.310	28.818	1.00 29.54	CPS6
ATOM	4903	CB	ARG	32	36.290	51.626	28.091	1.00 32.98	CPS6
ATOM	4904	CG	ARG	32	36.198	52.721	27.040	1.00 38.34	CPS6
ATOM	4905	CD	ARG	32	37.595	53.116	26.557	1.00 42.64	
ATOM	4906	NE	ARG	32	38.282	53.110	27.513		CPS6
								1.00 45.62	CPS6
ATOM	4907	CZ	ARG	32	38.009	55.281	27.677	1.00 47.09	CPS6
ATOM	4908		ARG	32	37.065	55.865	26.946	1.00 48.54	CPS6
ATOM	4909		ARG	32	38.675	55.992	28.576	1.00 48.16	CPS6
MOTA	4910	С	ARG	32	33.879	50.928	27.815	1.00 28.32	CPS6
ATOM	4911	0	ARG	32	32.969	51.711	27.544	1.00 27.76	CPS6
ATOM	4912	N	SER	33	33.966	49.719	27.275	1.00 27.75	CPS6
ATOM	4913	CA	SER	33	32.988	49.238	26.303	1.00 28.81	CPS6
ATOM	4914	CB	SER	33	33.386	47.828	25.835	1.00 30.61	CPS6
ATOM	4915	OG	SER	33	32.421	47.266	24.963	1.00 33.62	CPS6
ATOM	4916	C	SER	33	31.586	49.211	26.926	1.00 33.82	
ATOM	4917	ō	SER	33	30.599	49.614			CPS6
ATOM	4918	N					26.302	1.00 28.74	CPS6
ATOM			GLU	34	31.508	48.733	28.160	1.00 26.50	CPS6
	4919	CA	GLU	34	30.237	48.650	28.866	1.00 27.17	CPS6
ATOM	4920	CB	GLU	34	30.405	47.814	30.137	1.00 25.92	CPS6
ATOM	4921	CG	GLU	34	30.649	46.339	29.830	1.00 25.85	CPS6
ATOM	4922	CD	GLU	34	30.989	45.521	31.064	1.00 25.48	CPS6
ATOM	4923	OE1	GLU	34	30.771	44.290	31.035	1.00 24.91	CPS6
ATOM	4924	OE2	GLU	34	31.479	46.102	32.057	1.00 23.64	CPS6
ATOM	4925	С	GLU	34	29.688	50.029	29.193	1.00 27.92	CPS6
ATOM	4926	0	GLU	34	28.492	50.276	29.026	1.00 28.34	CPS6
ATOM	4927	N	LEU	35	30.556	50.929	29.648	1.00 27.84	CPS6
ATOM	4928	CA	LEU	35	30.137	52.286	29.977		
ATOM	4929	CB	LEU	35	31.310			1.00 30.69	CPS6
ATOM	4930	CG	LEU			53.081	30.557	1.00 30.33	CPS6
ATOM				35	31.719	52.712	31.981	1.00 30.63	CPS6
	4931		LEU	35	33.062	53.354	32.327	1.00 30.22	CPS6
ATOM	4932		LEU	35	30.631	53.170	32.943	1.00 30.10	CPS6
ATOM	4933	С	LEU	35	29.583	53.012	28.756	1.00 32.12	CPS6
ATOM	4934	0	LEU	35	28.669	53.826	28.880	1.00 32.67	CPS6
ATOM	4935	N	ASP	36	30.140	52.730	27.579	1.00 34.02	CPS6
ATOM	4936	CA	ASP	36	29.656	53.376	26.362	1.00 36.28	CPS6
ATOM	4937	CB	ASP	36	30.457	52.928	25.131	1.00 38.02	CPS6
ATOM	4938	CG	ASP	36	31.801	53.636	25.016	1.00 41.17	CPS6
ATOM	4939	OD1	ASP	36	31.924	54.767	25.538	1.00 42.30	CPS6
ATOM	4940		ASP	36	32.730	53.073	24.391	1.00 43.23	
ATOM	4941	C	ASP	36	28.177	53.073			CPS6
ATOM	4942	ŏ	ASP	36	27.411		26.152	1.00 37.04	CPS6
ATOM	4943	N	GLN			53.945	25.756	1.00 38.21	CPS6
ATOM	4943			37	27.772	51.836	26.427	1.00 36.14	CPS6
		CA	GLN	37	26.376	51.449	26.261	1.00 37.10	CPS6
ATOM	4945	CB	GLN	37	26.253	49.928	26.271	1.00 39.04	CPS6
ATOM	4946	CG	GLN	37	27.296	49.234	25.424	1.00 43.60	CPS6
ATOM	4947	CD	GLN	37	27.084	47.741	25.357	1.00 47.47	CPS6
ATOM	4948	OE1	GLN	37	26.134	47.268	24.726	1.00 50.58	CPS6
ATOM	4949	NE2	GLN	37	27.960	46.983	26.016	1.00 47.62	CPS6
ATOM	4950	C	GLN	37	25.535	52.042	27.389	1.00 36.39	CPS6
ATOM	4951	0	GLN	37	24.466	52.607	27.159	1.00 36.41	CPS6
ATOM	4952	N	TYR	38	26.045	51.909	28.608	1.00 35.09	CPS6
ATOM	4953	CA	TYR	38					
ATOM	4954	CB	TYR		25.395	52.405	29.813	1.00 35.03	CPS6
ATOM				38	26.346	52.199	31.000	1.00 33.56	CPS6
	4955	CG	TYR	38	25.868	52.724	32.330	1.00 32.55	CPS6
ATOM	4956		TYR	38	26.296	53.958	32.810	1.00 32.33	CPS6
ATOM	4957		TYR	38	25.882	54.427	34.057	1.00 33.78	CPS6
MOTA	4958	CD2	TYR	38	25.008	51.969	33.127	1.00 31.82	CPS6

FIG. 1A-86



SEP 0 9 2002 **TECH CENTER 1600/2900**

CPS6

FIG. 1A-87

SUBCLASS ci 2.9

3001								
ATOM	4959	CE2		38	24.590	52.423	34.367	1.00 32.17
ATOM	4960	CZ	TYR	38	25.029	53.652	34.829	1.00 33.51
ATOM	4961	OH	TYR	38	24.611	54.099	36.060	1.00 34.37
ATOM	4962	C	TYR	38	24.978	53.872	29.714	1.00 36.19
ATOM	4963	0	TYR	38	23.825	54.213	29.974	1.00 35.32
ATOM	4964	N	TYR	39	25.917	54.733	29.335	1.00 37.73
ATOM	4965	CA	TYR	39	25.649	56.168	29.229	1.00 37.73
ATOM	4966	CB	TYR	39	26.922	56.925	28.838	
ATOM	4967	CG	TYR	39	28.029	56.896		1.00 39.88
ATOM	4968		TYR	39	27.742		29.873	1.00 40.44
ATOM	4969	CE1		39		56.963	31.239	1.00 39.77
ATOM	4970	CD2			28.762	56.991	32.188	1.00 39.44
ATOM	4971	CE2		39	29.370	56.855	29.481	1.00 40.21
ATOM	4972			39	30.399	56.884	30.420	1.00 39.93
		CZ	TYR	39	30.089	56.954	31.773	1.00 40.43
ATOM	4973	OH	TYR	39	31.109	57.010	32.702	1.00 40.54
ATOM	4974	C.	TYR	39	24.538	56.54 6	28.254	1.00 41.06
ATOM	4975	0	TYR	39	23.957	57.627	28.357	1.00 42.29
ATOM	4976	N	GLU	40	24.239	55.668	27.307	1.00 42.33
MOTA	4977	CA	GLU	40	23.199	55.965	26.331	1.00 44.33
ATOM	4978	CB	GLU	40	23.541	55.323	24.986	1.00 46.05
ATOM	4979	CG	GLU	40	24.916	55.689	24.466	1.00 50.15
ATOM	4980	CD	GLU	40	25.203	55.088	23.105	1.00 52.92
ATOM	4981	OE1	GLU	40	25.040	53.857	22.948	1.00 55.32
ATOM	4982	OE2	GLU	40	25.599	55.848	22.191	1.00 54.91
ATOM	4983	С	GLU	40	21.827	55.488	26.780	
ATOM	4984	0	GLU	40	20.854	55.629		1.00 44.19
ATOM	4985	N	LEU	41	21.743	54.941	26.041	1.00 44.77
ATOM	4986	CA	LEU	41			27.991	1.00 42.63
ATOM	4987	CB	LEU	41	20.474	54.427	28.499	1.00 42.23
ATOM	4988	CG	LEU		20.696	53.114	29.259	1.00 41.12
ATOM	4989			41	21.294	51.934	28.486	1.00 40.93
ATOM		CD1	LEU	41	21.524	50.777	29.446	1.00 39.97
	4990	CD2	LEU	41	20.362	51.514	27.360	1.00 40.04
ATOM	4991	C	LEU	41	19.736	55.392	29.410	1.00 41.84
ATOM	4992	0	LEU	41	20.317	56.335	29.934	1.00 41.86
ATOM	4993	N	SER	42	18.447	55.129	29.597	1.00 42.32
ATOM	4994	CA	SER	42	17.602	55.937	30.465	1.00 43.65
ATOM	4995	CB	SER	42	16.134	55.578	30.252	1.00 43.85
ATOM	4996	OG	SER	42	15.871	54.269	30.726	1.00 44.29
ATOM	4997	C	SER	42	17.983	55.620	31.902	1.00 43.88
ATOM	4998	0	SER	42	18.661	54.626	32.157	1.00 44.22
ATOM	4999	N	GLU	43	17.540	56.447	32.843	1.00 44.22
ATOM	5000	CA	GLU	43	17.860	56.216	34.248	
ATOM	5001	CB	GLU	43	17.195	57.266		1.00 44.69
ATOM	5002	CG	GLU	43	17.466		35.147	1.00 47.52
ATOM	5003	CD	GLU	43		57.033	36.632	1.00 51.04
ATOM	5004	OE1	GLU	43	16.733	58.002	37.54 6	1.00 53.92
ATOM	5005		GLU		15.480	57.965	37.596	1.00 55.09
ATOM	5006	C	GLU	43	17.418	58.802	38.221	1.00 55.13
ATOM	5007			43	17.411	54.828	34.687	1.00 43.76
		0	GLU	43	18.123	54.143	35.419	1.00 43.62
ATOM	5008	N	LYS	44	16.227	54.419	34.244	1.00 42.65
ATOM	5009	CA	LYS	44	15.699	53.110	34.601	1.00 42.18
ATOM	5010	CB	LYS	44	14.244	52.980	34.151	1.00 43.86
ATOM	5011	CG	LYS	44	13.612	51.643	34.508	1.00 45.75
ATOM	5012	CD	LYS	44	12.155	51.590	34.086	1.00 47.40
ATOM	5013	CE	LYS	44	11.521	50.267	34.474	1.00 48.83
ATOM	5014	NZ	LYS	44	10.076	50.213	34.107	1.00 50.91
ATOM	5015	C	LYS	44	16.521	51.994	33.966	1.00 40.95
							-5.500	1.00 40.95



SEP 0 9 2002

FIG. 1A-88

:16.	SUBCLASS	
0.0	CLASS	
APPAOVEU	*8	DRAFTSMAH

ATOM	5016	0	LYS	44	16.952	51.064	34.645	1.00 40.09	CPS6
MOTA	5017	N	ARG	45	16.722	52.091	32.656	1.00 39.93	CPS6
ATOM	5018	CA	ARG	45	17.490	51.095	31.923	1.00 38.26	CPS6
ATOM	5019	CB	ARG	45	17.518	51.437	30.434	1.00 40.94	CPS6
ATOM	5020	CG	ARG	45	16.178	51.285	29.736	1.00 45.37	CPS6
ATOM	5021	CD	ARG	45	15.796	49.825	29.572	1.00 48.47	CPS6
ATOM	5022	NE	ARG	45	16.746	49.092	28.732	1.00 52.03	CPS6
ATOM	5023	CZ	ARG	45	17.047	49.411	27.475	1.00 54.07	CPS6
ATOM	5024	NH1	ARG	45	16.480	50.459	26.888	1.00 55.15	CPS6
ATOM	5025	NH2	ARG	45	17.917	48.672	26.796	1.00 55.63	CPS6
ATOM	5026	С	ARG	45	18.915	50.992	32.441	1.00 35.74	CPS6
ATOM	5027	0	ARG	45	19.524	49.926	32.374	1.00 33.44	CPS6
ATOM	5028	N	LYS	46	19.456	52.098	32.945	1.00 33.77	CPS6
MOTA	5029	CA	LYS	46	20.814	52.075	33.466	1.00 32.86	CPS6
MOTA	5030	CB	LYS	46	21.311	53.489	33.787	1.00 32.65	CPS6
ATOM	5031	CG	LYS	46	21.636	54.270	32.529	1.00 35.15	CPS6
ATOM	5032	CD	LYS	46	22.700	55.318	32.752	1.00 38.55	
ATOM	5033	CE	LYS	46	22.185	56.492	33.528	1.00 38.97	CPS6
ATOM	5034	NZ	LYS	46	22.923	57.716	33.328	1.00 40.88	
ATOM	5035	C	LYS	46	20.904	51.196	34.693	1.00 40.88	CPS6
ATOM	5036	ō	LYS	46	21.841	50.415			CPS6
ATOM	5037	N	ASN	47	19.927	51.310	34.832	1.00 30.69	CPS6
ATOM	5038	CA	ASN	47	19.935	50.486	35.585	1.00 30.34	CPS6
ATOM	5039	СВ	ASN	47	18.779	50.880	36.788	1.00 29.82	CPS6
ATOM	5040	CG	ASN	47	18.683	49.983	37.713	1.00 30.59	CPS6
ATOM	5041		ASN	47	19.510		38.935	1.00 32.30	CPS6
ATOM	5042		ASN	47	17.675	50.057	39.851	1.00 33.45	CPS6
ATOM	5042	C	ASN	47		49.119	38.950	1.00 34.07	CPS6
ATOM	5044	ō	ASN	47	19.821	49.003	36.401	1.00 28.64	CPS6
ATOM	5045	N	GLU	48		48.154	36.970	1.00 28.65	CPS6
ATOM	5046	CA	GLU	48	18.972	48.700	35.424	1.00 28.08	CPS6
ATOM	5047	CB	GLU	48	18.796	47.319	34.969	1.00 28.15	CPS6
ATOM	5048	CG	GLU	48	17.680	47.234	33.927	1.00 31.68	CPS6
ATOM	5049	CD	GLU	48	16.301	47.618	34.448	1.00 36.94	CPS6
ATOM	5050		GLU	48	15.246	47.631	33.352	1.00 40.49	CPS6
ATOM	5051		GLU	48	14.076	47.950	33.661	1.00 42.57	CPS6
ATOM	5052	C	GLU	48	15.585	47.325	32.185	1.00 40.94	CPS6
ATOM	5053	ò	GLU	48	20.085	46.783	34.344	1.00 27.02	CPS6
ATOM	5054	N	PHE		20.489	45.646	34.598	1.00 25.06	CPS6
ATOM	5055	CA	PHE	49	20.714	47.613	33.515	1.00 25.48	CPS6
ATOM	5056	CB	PHE	49	21.949	47.243	32.830	1.00 26.00	CPS6
ATOM	5057	CG	PHE	49	22.351	48.358	31.858	1.00 26.69	CPS6
ATOM	5058			49	23.585	48.058	31.057	1.00 27.23	CPS6
ATOM	5059		PHE	49	23.497	47.397	29.838	1.00 28.29	CPS6
ATOM	5060		PHE	49	24.835	48.455	31.515	1.00 26.82	CPS6
ATOM	5061		PHE	49	24.640	47.142	29.081	1.00 28.93	CPS6
ATOM	5062	CZ		49	25.987	48.202	30.765	1.00 27.94	CPS6
ATOM	5062		PHE	49	25.886	47.548	29.550	1.00 28.38	CPS6
ATOM	5064	C	PHE	49	23.066	46.997	33.837	1.00 24.84	CPS6
ATOM		0	PHE	49	23.739	45.966	33.789	1.00 25.50	CPS6
ATOM	5065 5066	N	LEU	50	23.264	47.946	34.747	1.00 24.16	CPS6
ATOM		CA	LEU	50	24.296	47.824	35.773	1.00 22.97	CPS6
ATOM	5067	CB	LEU	50	24.304	49.088	36.647	1.00 24.37	CPS6
	5068	CG	LEU	50	25.348	49.178	37.759	1.00 25.79	CPS6
ATOM	5069	CD1		50	26.760	49.145	37.149	1.00 26.03	CPS6
ATOM	5070	CD2		50	25.141	50.471	38.537	1.00 26.29	CPS6
ATOM	5071	С	LEU	50	24.081	46.583	36.653	1.00 21.87	CPS6
ATOM	5072	0	LEU	50	25.022	45.839	36.939	1.00 21.43	CPS6



RECEIVED SEP 0 9 2002

FIG. 1A-89

cj	SUBCLASS	
0.6. FI	CLASS SI	
APPROVED	2-	DRAFTSMAH

ATOM	5073	N	ALA	51	22.844	46.364	37.089	1.00 21.05	CPS6
ATOM	5074	CA	ALA	51	22.524	45.218	37.940	1.00 21.01	CPS6
ATOM	5075	CB	ALA	51	21.038	45.271	38.346	1.00 20.12	CPS6
MOTA	5076	C	ALA	51	22.829	43.894	37.223	1.00 20.25	CPS6
ATOM	5077	0	ALA	51	23.351	42.955	37.825	1.00 20.85	CPS6
ATOM	5078	N	GLY	52	22.493	43.830	35.943	1.00 21.02	CPS6
ATOM	5079	CA	GLY	52	22.742	42.624	35.164	1.00 20.99	CPS6
ATOM	5080	С	GLY	52	24.232	42.376	34.989	1.00 22.24	CPS6
MOTA	5081	0	GLY	52	24.688	41.232	35.044	1.00 21.77	CPS6
ATOM	5082	N	ARG	53	24.992	43.444	34.764	1.00 22.45	CPS6
MOTA	5083	CA	ARG	53	26.442	43.317	34.600	1.00 22.02	CPS6
ATOM	5084	CB	ARG	53	27.051	44.624	34.093	1.00 23.58	CPS6
ATOM	5085	CG	ARG	53	26.831	44.875	32.628	1.00 26.56	CPS6
ATOM	5086	CD	ARG	53	27.406	43.749	31.834	1.00 28.57	CPS6
MOTA	5087	NE	ARG	53	27.764	44.164	30.483	1.00 32.59	CPS6
ATOM	5088	CZ	ARG	53	26.903	44.301	29.481	1.00 32.51	CPS6
ATOM	5089	NH1	ARG	53	25.606	44.053	29.676	1.00 29.51	CPS6
ATOM	5090	NH2	ARG	53	27.352	44.666	28.277	1.00 29.31	CPS6
ATOM	5091	C	ARG	53	27.081	42.951	35.926	1.00 22.03	CPS6
ATOM	5092	0	ARG	53	28.014	42.159	35.983	1.00 22.12	CPS6
ATOM	5093	N	PHE	54	26.576	43.541	37.000	1.00 20.72	CPS6
ATOM	5094	CA	PHE	54	27.089	43.253	38.322	1.00 21.84	CPS6
ATOM	5095	CB	PHE	54	26.391	44.144	39.347	1.00 23.57	CPS6
ATOM	5096	CG	PHE	54	26.843	43.925	40.756	1.00 24.76	CPS6
ATOM	5097	CD1		54	26.202	42.996	41.571	1.00 26.78	CPS6
MOTA	5098	CD2		54	27.896	44.666	41.282	1.00 26.87	CPS6
MOTA	5099	CE1		54	26.603	42.815	42.886	1.00 27.91	CPS6
MOTA	5100	CE2	PHE	54	28.302	44.491	42.592	1.00 26.99	CPS6
ATOM	5101	CZ	PHE	54	27.656	43.567	43.397	1.00 27.41	CPS6
ATOM	5102	С	PHE	54	26.865	41.777	38.647	1.00 21.21	CPS6
ATOM	5103	0	PHE	54	27.768	41.097	39.123	1.00 20.78	CPS6
ATOM	5104	N	ALA	55	25.665	41.277	38.381	1.00 20.89	CPS6
ATOM	5105	CA	ALA	55	25.374	39.872	38.669	1.00 20.22	CPS6
ATOM	5106	CB	ALA	55	23.892	39.574	38.441	1.00 19.35	CPS6
ATOM	5107	С	ALA	55	26.224	38.955	37.805	1.00 18.66	CPS6
ATOM	5108	0	ALA	55	26.716	37.923	38.278	1.00 19.74	CPS6
ATOM	5109	N	ALA	56	26.395	39.314	36.538	1.00 18.06	CPS6
ATOM	5110	CA	ALA	56	27.195	38.488	35.639	1.00 18.21	CPS6
ATOM	5111	CB	ALA	56	27.134	39.041	34.198	1.00 18.23	CPS6
ATOM	5112	С	ALA	56	28.648	38.387	36.101	1.00 18.83	CPS6
ATOM	5113	0	ALA	56	29.259	37.307	36.057	1.00 17.66	CPS6
ATOM	5114	N	LYS	57	29.207	39.508	36.549	1.00 19.03	CPS6
ATOM	5115	CA	LYS	57	30.592	39.513	37.012	1.00 18.37	CPS6
ATOM	5116	CB	LYS	57	31.101	40.958	37.085	1.00 19.18	CPS6
ATOM	5117	CG	LYS	57	31.179	41.574	35.689	1.00 19.49	CPS6
ATOM	5118	CD	LYS	57	31.775	42.975	35.676	1.00 23.00	CPS6
ATOM	5119	CE	LYS	57	31.663	43.579	34.285	1.00 20.60	CPS6
ATOM	5120	NZ	LYS	57	32.580	44.729	34.103	1.00 21.27	CPS6
ATOM	5121	C	LYS	57	30.745	38.785	38.344	1.00 19.47	CPS6
ATOM	5122	0	LYS	57	31.739	38.084	38.557	1.00 20.88	CPS6
ATOM	5123	N	GLU	58	29.773	38.942	39.245	1.00 19.43	CPS6
MOTA	5124	CA	GLU	58	29.821	38.212	40.512	1.00 21.77	CPS6
ATOM	5125	CB	GLU	58	28.640	38.591	41.419	1.00 22.85	CPS6
MOTA	5126	CG	GLU	58	28.746	39.965	42.066	1.00 27.74	CPS6
ATOM	5127	CD	GLU	58	29.884	40.060	43.079	1.00 30.88	CPS6
ATOM	5128	OE1		58	30.148	41.173	43.580	1.00 34.74	CPS6
ATOM	5129	OE2	GLU	58	30.517	39.028	43.378	1.00 34.50	CPS6



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 1A-90

·	T.O.	
FIG.	SUBCLASS	
0.00	CLASS	*
APPROVE	>- Ga	ORAFISHA

ATOM	5130	C	GLU	58	29.745	36.711	40.199	1.00 21.81	CPS6
MOTA	5131	0	GLU	58	30.494	35.90 0	40.767	1.00 21.58	CPS6
ATOM	5132	N	ALA	59	28.833	36.332	39.305	1.00 20.31	CPS6
MOTA	5133	CA	ALA	59	28.704	34.917	38.958	1.00 20.01	CPS6
MOTA	5134	CB	ALA	59	27.557	34.709	37.956	1.00 19.39	CPS6
MOTA	5135	C	ALA	59	30.015	34.398	38.370	1.00 20.62	CPS6
MOTA	5136	0	ALA	59	30.463	33.289	38.693	1.00 21.08	CPS6
ATOM	5137	И	PHE	60	30.625	35.192	37.497	1.00 18.52	CPS6
MOTA	5138	CA	PHE	60	31.886	34.784	36.891	1.00 20.21	CPS6
ATOM	5139	CB	PHE	60	32.359	35.819	35.863	1.00 19.79	CPS6
ATOM	5140	CG	PHE	60	33.690	35.482	35.248	1.00 21.99	CPS6
ATOM	5141	CD1		60	33.768	34.653	34.133	1.00 19.74	CPS6
MOTA	5142	CD2		60	34.874	35.925	35.842	1.00 22.16	CPS6
MOTA	5143	CE1		60	35.010	34.264	33.618	1.00 23.98	CPS6
ATOM	5144	CE2		60	36.117	35.542	35.339	1.00 23.86	CPS6
ATOM	5145	CZ	PHE	60	36.187	34.709	34.227	1.00 23.24	CPS6
ATOM	5146	C	PHE	60	32.970	34.614	37.961	1.00 21.37	CPS6
ATOM	5147	0	PHE	60	33.724	33.638	37.938	1.00 22.00	CPS6
ATOM	5148	N	SER	61	33.048	35.565	38.891	1.00 21.71	CPS6
ATOM	5149	CA	SER	61	34.065	35.516	39.945	1.00 23.80	CPS6
ATOM	5150	CB	SER	61	34.003	36.772	40.824	1.00 23.70	CPS6
ATOM	5151	OG	SER	61	32.938	36.694	41.753	1.00 25.60	CPS6
ATOM	5152	C	SER	61	33.912	34.284	40.824	1.00 24.14	CPS6
ATOM	5153	0	SER	61	34.897	33.786	41.386	1.00 25.44	CPS6
ATOM	5154	И	LYS	62	32.683	33.800	40.957	1.00 23.98	CPS6
MOTA	5155	CA	LYS	62	32.425	32.609	41.764	1.00 25.63	CPS6
ATOM	5156	CB	LYS	62	30.946	32.566	42.174	1.00 25.79	CPS6
ATOM	5157	CG	LYS	62	30.601	33.735	43.097	1.00 29.14	CPS6
ATOM	5158	CD	LYS	62	29.112	33.966	43.281	1.00 32.29	CPS6
ATOM	5159	CE	LYS	62	28.492	32.995	44.255	1.00 34.95	CPS6
ATOM	5160	NZ	LYS	62	27.224	33.584	44.793	1.00 38.32	CPS6
ATOM	5161	С	LYS	62	32.830	31.358	40.995	1.00 26.22	CPS6
ATOM	5162	0	LYS	62	33.397	30.424	41.568	1.00 25.89	CPS6
ATOM	5163	И	ALA	63	32.556	31.343	39.693	1.00 24.67	CPS6
MOTA	5164	CA	ALA	63	32.936	30.209	38.861	1.00 24.83	CPS6
ATOM	5165	CB	ALA	63	32.345	30.359	37.464	1.00 24.34	CPS6
ATOM	5166	C	ALA	63	34.459	30.174	38.780	1.00 26.66	CPS6
MOTA	5167	0	ALA	63	35.064	29.105	38.737	1.00 26.11	CPS6
ATOM ATOM	5168	N	PHE	64	35.071	31.354	38.762	1.00 26.12	CPS6
ATOM	5169	CA	PHE	64	36.526	31.467	38.692	1.00 28.50	CPS6
ATOM	5170 5171	CB	PHE	64	36.919	32.925	38.445	1.00 28.06	CPS6
ATOM	5172		PHE	64 64	38.341	33.104	37.992	1.00 29.52	CPS6 CPS6
ATOM	5172	CD2	PHE	64	38.760	32.606	36.765	1.00 29.61	
ATOM	5174		PHE		39.251	33.787	38.787	1.00 29.01	CPS6
ATOM	5175		PHE	64 64	40.072	32.787	36.329	1.00 32.11 1.00 30.85	CPS6 CPS6
ATOM	5176	CZ	PHE	64	40.565	33.973 33.473	38.362 37.130	1.00 30.85	CPS6
ATOM	5177	c	PHE	64				1.00 31.27	CPS6
ATOM	5178	0	PHE	64	37.176 38.376	30.953	39.981	1.00 29.90	CPS6
ATOM	5179	и	GLY	65		30.661	40.003	1.00 30.91	CPS6
ATOM	5180	CA	GLY	65	36.377	30.858	41.043	1.00 31.52	CPS6
ATOM	5181	CA	GLY	65	36.845 37.435	30.349	42.322	1.00 34.23	CPS6
ATOM	5182	0	GLY	65	37.435	31.337	44.456	1.00 36.45	CPS6
ATOM	5183	Ŋ	THR	66	37.726	30.968	44.456	1.00 37.62	CPS6
ATOM	5184	CA	THR	66	37.593		42.902	1.00 36.65	CPS6
ATOM	5185	CB	THR	66	39.272	33.616	43.755	1.00 36.52	CPS6
ATOM	5186	OG1	THR	66	39.272	34.385	42.978	1.00 36.32	CPS6



SEP 0 9 2002

FIG. 1A-91

FIG.	SUBCLASS	
.10.6.	CLASS	3
APPLOYER	34	DRAFTSHAN

N MONE	F 7 0 7	000	mith	66	40 207	33.429	42.389	1 00 36 70	anac
ATOM	5187	CG2			40.297			1.00 36.79	CPS6
ATOM	5188	С	THR	66	37.243	34.666	44.329	1.00 36.19	CPS6
ATOM	5189	0	THR	66	37.475	35.193	45.419	1.00 35.77	CPS6
ATOM	5190	И	GLY	67	36.175	34.973	43.599	1.00 35.09	CPS6
ATOM	5191	CA	GLY	67	35.266	36.011	44.046	1.00 33.07	CPS6
ATOM	5192	C	GLY	67	35.944	37.308	43.634	1.00 32.90	CPS6
ATOM	5193	0	GLY	67	37.083	37.269	43.168	1.00 32.07	CPS6
ATOM	5194	N	ILE	68	35.264	38.446	43.766	1.00 32.48	CPS6
ATOM	5195	CA	ILE	68	35.878	39.721	43.397	1.00 32.14	CPS6
ATOM	5196	CB	ILE	68	34.821	40.823	43.170	1.00 31.75	CPS6
		CG2		68	35.509	42.167	42.928	1.00 32.21	CPS6
ATOM	5197								
ATOM	5198	CG1		68	33.941	40.463	41.967	1.00 30.11	CPS6
ATOM	5199	CD1		68	34.697	40.354	40.642	1.00 30.32	CPS6
ATOM	5200	С	ILE	68	36.796	40.150	44.536	1.00 33.67	CPS6
ATOM	5201	0	ILE	68	36.370	40.206	45.692	1.00 33.24	CPS6
ATOM	5202	N	GLY	69	38.050	40.443	44.207	1.00 34.42	CPS6
ATOM	5203	CA	GLY	69	39.002	40.845	45.226	1.00 37.25	CPS6
ATOM	5204	С	GLY	69	40.431	40.946	44.719	1.00 38.28	CPS6
ATOM	5205	0	GLY	69	40.669	41.302	43.567	1.00 38.30	CPS6
ATOM	5206	N	ALA	70	41.386	40.609	45.579	1.00 38.96	CPS6
ATOM	5207	CA	ALA	70	42.800	40.684	45.233	1.00 39.69	CPS6
ATOM	5208	CB	ALA	70	43.644	40.198	46.415	1.00 40.64	CPS6
ATOM	5209	C	ALA	70	43.208	39.939	43.965	1.00 39.83	CPS6
ATOM	5210	0	ALA	70	44.175	40.322	43.311	1.00 40.54	CPS6
ATOM	5211	N	GLN	71	42.481	38.885	43.605	1.00 39.94	CPS6
ATOM	5212	CA	GLN	71	42.834	38.115	42.411	1.00 39.34	CPS6
MOTA	5213	CB	GLN	71	42.773	36.614	42.709	1.00 41.56	CPS6
MOTA	5214	CG	GLN	71	43.429	36.181	44.006	1.00 43.98	CPS6
ATOM	5215	CD	GLN	71	43.299	34.684	44.233	1.00 45.96	CPS6
ATOM	5216	OE1	GLN	71	43.901	33.880	43.515	1.00 48.14	CPS6
ATOM	5217	NE2	GLN	71	42.502	34.302	45.224	1.00 46.92	CPS6
ATOM	5218	C	GLN	71	41.972	38.381	41.176	1.00 37.54	CPS6
ATOM	5219	0	GLN	71	42.286	37.886	40.096	1.00 37.40	CPS6
ATOM	5220	N	LEU	72	40.898	39.154	41.326	1.00 35.40	CPS6
ATOM	5221	CA	LEU	72	39.998	39.428	40.204	1.00 33.24	CPS6
ATOM	5222	CB	LEU	72	39.029	38.257	40.026	1.00 31.49	CPS6
ATOM	5223	CG	LEU	72	38.647	37.600	38.692	1.00 32.42	CPS6
ATOM	5224		LEU	72	37.168	37.243	38.788	1.00 32.42	CPS6
ATOM								1.00 28.80	CPS6
	5225		LEU	72 .	38.919	38.478	37.487		
ATOM	5226	С	LEU	72	39.174	40.680	40.483	1.00 31.78	CPS6
ATOM	5227	0	LEU	72	38.496	40.758	41.502	1.00 32.54	CPS6
ATOM	5228	14	SER	73	39.217	41.652	39.583	1.00 30.85	CPS6
ATOM	5229	CA	SER	73	38.428	42.866	39.784	1.00 29.39	CPS6
ATOM	5230	CB	SER	73	39.289	44.113	39.615	1.00 30.61	CPS6
ATOM	5231	OG	SER	73	39.523	44.366	38.246	1.00 30.25	CPS6
ATOM	5232	C -	SER	73	37.309	42.898	38.752	1.00 27.96	CPS6
ATOM	5233	0	SER	73	37.333	42.147	37.775	1.00 27.49	CPS6
ATOM	5234	N	PHE	74	36.322	43.760	38.975	1.00 26.79	CPS6
ATOM	5235	CA	PHE	74	35.213	43.888	38.034	1.00 26.21	CPS6
ATOM	5236	CB	PHE	74	34.219	44.938	38.534	1.00 25.48	CPS6
ATOM	5237	CG	PHE	74	33.366			1.00 26.75	CPS6
						44.472	39.676		
ATOM	5238		PHE	74	32.329	43.568	39.460	1.00 27.07	CPS6
MOTA	5239		PHE	74	33.582	44.949	40.967	1.00 27.57	CPS6
ATOM	5240		PHE	74	31.511	43.148	40.515	1.00 27.84	CPS6
ATOM	5241		PHE	74	32.770	44.534	42.030	1.00 28.92	CPS6
ATOM	5242	CZ	PHE	74	31.732	43.634	41.801	1.00 27.85	CPS6
MOTA	5243	С	PHE	74	35.731	44.301	36.659	1.00 26.17	CPS6



SEP 0 9 2002

FIG. 1A-92

.F1G.	S SUBCLASS	
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ATOM	5244	0	PHE	74	35.186	43.903	35.638	1.00 25.99	CPS6
ATOM	5245	N	GLN	75	36.793	45.103	36.638	1.00 25.96	CPS6
ATOM	5246	CA	GLN	75	37.365	45.583	35.384	1.00 27.32	CPS6
ATOM	5247	CB	GLN	75	38.374	46.703	35.665	1.00 27.52	CPS6
ATOM	5248	CG	GLN	75	37.754	47.960	36.271	1.00 30.15	CPS6
ATOM	5249	CD	GLN	75	36.770	48.648	35.339	1.00 30.80	CPS6
ATOM	5250		GLN	75	37.052	48.857	34.159	1.00 31.37	CPS6
ATOM	5251		GLN	75	35.618	49.019	35.871	1.00 34.02	CPS6
ATOM	5252	С	GLN	75	38.024	44.498	34.530	1.00 26.97	CPS6
ATOM	5253	ō	GLN	75	38.199	44.679	33.329	1.00 26.86	CPS6
ATOM	5254	N	ASP	76	38.382	43.377	35.150	1.00 27.98	CPS6
ATOM	5255	CA	ASP	76	39.004	42.258	34.437	1.00 27.78	CPS6
ATOM	5256	CB	ASP	76	39.644	41.271	35.421	1.00 27.70	CPS6
ATOM	5257	CG	ASP	76	40.883	41.813	36.091	1.00 23.30	CPS6
ATOM	5258		ASP	76	41.690	42.457	35.397	1.00 35.07	CPS6
ATOM	5259		ASP	76	41.059	41.570	37.307	1.00 32.81	CPS6
ATOM	5260	C	ASP	76	37.969	41.474	33.633	1.00 32.81	CPS6
			ASP	76					
ATOM	5261	0			38.314	40.671	32.764	1.00 26.16	CPS6
ATOM	5262	N	ILE	77	36.696	41.705	33.930	1.00 26.25	CPS6
ATOM	5263	CA	ILE	77	35.616	40.966	33.272	1.00 25.67	CPS6
ATOM	5264	CB	ILE	77	34.682	40.360	34.335	1.00 25.40	CPS6
MOTA	5265			77	33.688	39.404	33.681	1.00 24.95	CPS6
ATOM	5266		ILE	77	35.511	39.639	35.400	1.00 23.36	CPS6
MOTA	5267		ILE	77	34.798	39.549	36.758	1.00 23.84	CPS6
MOTA	5268	C	ILE	77	34.785	41.871	32.372	1.00 25.23	CPS6
MOTA	5269	0	ILE	77	34.326	42.916	32.809	1.00 26 .6 6	CPS6
ATOM	5270	1/1	GLU	78	34.579	41.473	31.123	1.00 24.36	CPS6
MOTA	5271	CA	GLU	78	33.794	42.296	30.217	1.00 23.95	CPS6
MOTA	5272	CB	GLU	78	34.689	42.928	29.151	1.00 23.23	CPS6
MOTA	5273	CG	GLU	78	33.936	43.867	28.231	1.00 25.47	CPS6
ATOM	5274	CD	GLU	78	34.858	44.740	27.406	1.00 28.41	CPS6
MOTA	5275		GLU	78	35.313	44.287	26.331	1.00 28.29	CPS6
ATOM	5276		GLU	78	35.133	45.880	27.844	1.00 29.93	CPS6
MOTA	5277	С	GLU	78	32.698	41.501	29.523	1.00 23.31	CPS6
ATOM	5278	0	GLU	78	32.951	40.411	29.013	1.00 23.66	CPS6
ATOM	5279	N	ILE	79	31.481	42.045	29.519	1.00 23.40	CPS6
ATOM	5280	CA	ILE	79	30.376	41.377	28.843	1.00 22.82	CPS6
MOTA	5281	CB	ILE	79	29.074	41.348	29.696	1.00 22.78	CPS6
ATOM	5282	CG2	ILE	79	27.899	40.913	28.834	1.00 23.83	CPS6
ATOM	5283	CG1	ILE	79	29.214	40.370	30.871	1.00 23.62	CPS6
ATOM	5284	CD1	ILE	79	29.978	40.908	32.041	1.00 26.29	CPS6
ATOM	5285	C	ILE	79	30.081	42.125	27.551	1.00 22.89	CPS6
ATOM	5286	0	ILE	79	29.992	43.352	27.547	1.00 21.79	CPS6
ATOM	5287	N	ARG	80	29.969	41.383	26.456	1.00 22.11	CPS6
ATOM	5288	CA	ARG	80	29.625	41.957	25.152	1.00 24.89	CPS6
ATOM	5289	CB	ARG	80	30.781	41.821	24.147	1.00 28.30	CPS6
ATOM	5290	CG	ARG	80	32.171	41.662	24.758	1.00 34.49	CPS6
ATOM	5291	CD	ARG	80	33.065	42.894	24.630	1.00 37.92	CPS6
ATOM	5292	NE	ARG	80	33.175	43.397	23.267	1.00 39.97	CPS6
ATOM	5293	CZ	ARG	80	34.078	44.291	22.857	1.00 39.55	CPS6
ATOM	5294		ARG	80	34.981	44.787	23.697	1.00 38.56	CPS6
ATOM	5295		ARG	80	34.050	44.724	21.604	1.00 37.96	CPS6
ATOM	5296	C	ARG	80	28.445	41.119	24.657	1.00 37.30	CPS6
ATOM	5297	ō	ARG	80	28.130	.40.095	25.249	1.00 24.70	CPS6
ATOM	5298	N	LYS	81	27.776		23.592	1.00 26.22	CPS6
ATOM	5299	CA	LYS	81	26.664	41.551		1.00 28.22	CPS6
ATOM	5300	CB	LYS	81		40.770	23.055		
22.014	2200	CB	212	91	25.346	41.547	23.140	1.00 30.47	CPS6



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FIG. 1A-93

TECH CENTER 1600/2900

MOTA	5301	CG	LYS	81	24.745	41.614	24.542	1.00 34.14	CPS6
MOTA	5302	CD	LYS	81	23.460	42.439	24.545	1.00 37.71	CPS6
MOTA	5303	CE	LYS	81	22.985	42.787	25.963	1.00 39.78	CPS6
ATOM	5304	NZ	LYS	81	22.435	41.636	26.736	1.00 39.75	CPS6
MOTA	5305	С	LYS	81	26.962	40.409	21.608	1.00 29.13	CPS6
MOTA	5306	0	LYS	81	27.536	41.222	20.876	1.00 29.46	CPS6
MOTA	5307	N	ASP	82	26.602	39.193	21.197	1.00 29.17	CPS6
MOTA	5308	CA	ASP	82	26.861	38.783	19.824	1.00 31.09	CPS6
ATOM	5309	CB	ASP	82	27.044	37,255	19.707	1.00 29.73	CPS6
ATOM	5310	CG	ASP	82	25.751	36.464	19.877	1.00 28.91	CPS6
ATOM	5311	OD1	ASP	82	24.646	37.045	19.861	1.00 26.18	CPS6
MOTA	5312	OD2	ASP	82	25.861	35.226	20.012	1.00 28.29	CPS6
ATOM	5313	C	ASP	82	25.775	39.283	18.891	1.00 31.70	CPS6
ATOM	5314	0	ASP	82	24.909	40.051	19.306	1.00 32.19	CPS6
MOTA	5315	N	GLN	83	25.821	38.852	17.634	1.00 35.43	CPS6
ATOM	5316	CA	GLN	83	24.854	39.300	16.634	1.00 37.80	CPS6
MOTA	5317	CB	GLN	83	25.222	38.738	15.252	1.00 40.89	CPS6
MOTA	5318	CG	GLN	83	25.267	37.219	15.164	1.00 44.70	CPS6
MOTA	5319	CD	GLN	83	26.534	36.612	15.755	1.00 47.79	CPS6
MOTA	5320	OE1		83	26.642	35.388	15.889	1.00 49.81	CPS6
ATOM	5321	NE2		83	27.503	37.461	16.101	1.00 48.69	CPS6
MOTA	5322	C	GLN	83	23.400	38.966	16.965	1.00 38.04	CPS6
MOTA	5323	0	GLN	83	22.481	39.641	16.499	1.00 38.72	CPS6
ATOM	5324	N	ASN	84	23.182	37.933	17.772	1.00 36.73	CPS6
MOTA	5325	CA	ASN	84	21.822	37.564	18.146	1.00 35.24	CPS6
ATOM	5326	CB	ASN	84	21.701	36.049	18.292	1.00 35.98	CPS6
MOTA	5327	CG	ASN	84	21.864	35.331	16.979	1.00 37.29	CPS6
MOTA	5328	OD1		84	21.242	35.699	15.977	1.00 39.43	CPS6
MOTA	5329	ND2		84	22.694	34.298	16.968	1.00 36.91	CPS6
MOTA	5330	С	ASN	84	21.400	38.234	19.447	1.00 33.77	CPS6
MOTA	5331	0	ASN	84	20.262	38.088	19.882	1.00 34.74	CPS6
MOTA	5332	N	GLY	85	22.322	38.963	20.067	1.00 31.96	CPS6
MOTA	5333	CA	GLY	85	22.011	39.635	21.315	1.00 30.32	CPS6
MOTA	5334	С	GLY	85	22.360	38.777	22.520	1.00 28.59	CPS6
MOTA	5335	0	GLY	85	22.022	39.112	23.655	1.00 28.08	CPS6
MOTA	5336	N	LYS	86	23.041	37.664	22.265	1.00 26.87	CPS6
ATOM	5337	CA	LYS	86	23.451	36.743	23.323	1.00 24.77	CPS6
MOTA	5338	CB	LYS	86	23.760	35.365	22.719	1.00 24.34	CPS6
MOTA	5339	CG	LYS	86	24.446	34.376	23.663	1.00 23.41	CPS6
ATOM ATOM	5340	CD	LYS	86	23.518	33.886	24.783	1.00 22.54	CPS6
ATOM	5341	CE	LYS	86	24.296	33.008	25.778	1.00 21.86	CPS6
ATOM	5342 5343	NZ	LYS	86	23.395	32.379	26.784	1.00 21.67	CPS6
ATOM	5344	C	LYS	86	24.690	37.282	24.028	1.00 23.40	CPS6
ATOM		0	LYS	86	25.709	37.558	23.390	1.00 22.20	CPS6
ATOM	5345 5346	N CD	PRO	87	24.628	37.443	25.359	1.00 22.90	CPS6
ATOM	5347	CA	PRO PRO	87	23.483	37.328	26.283	1.00 23.21	CPS6
ATOM	5347	CB	PRO	87	25.820	37.956	26.050	1.00 21.73	CPS6
ATOM	5349	CG	PRO	87	25.281	38.351	27.427	1.00 23.57	CPS6
MOTA	5350	C	PRO	87	24.166	37.350	27.648	1.00 23.73	CPS6
ATOM	5351	0	PRO	87	26.945	36.924	26.167	1.00 21.97	CPS6
ATOM	5352	N	TYR	87 88	26.693	35.724	26.260	1.00 19.28	CPS6
MOTA	5352	CA	TYR		28.192	37.393	26.124	1.00 21.22	CPS6
MOTA	5354	CB	TYR	88	29.333	36.504	26.308	1.00 20.65	CPS6
ATOM	5355	CG	TYR	88	29.881	35.972	24.980	1.00 22.01	CPS6
ATOM	5356	CD1			30.434	37.009	24.036	1.00 21.99	CPS6
ATOM	5357	CE1		88	31.796	37.317	24.021	1.00 25.46	CPS6
	233,		*11	00	32.310	38.251	23.121	1.00 24.59	CPS6



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FIG. 1A-94

ATOM	5358	CD2	TYR	88	29.600	37.666	23.132	1.00 25.11	CPS6
ATOM	5359	CE2	TYR	88	30.105	38.601	22.234	1.00 25.50	CPS6
ATOM	5360	CZ	TYR	88	31.459	38.887	22.235	1.00 26.13	CPS6
ATOM	5361	OH	TYR	88	31.947	39.824	21.351	1.00 28.03	CPS6
ATOM	5362	C	TYR	88	30.382	37.287	27.062	1.00 21.33	CPS6
ATOM	5363	0	TYR	88	30.415	38.512	27.009	1.00 22.02	CPS6
ATOM	5364	N	ILE	89	31.238	36.571	27.769	1.00 22.15	CPS6
ATOM	5365	CA	ILE	89	32.263	37.187	28.581	1.00 22.97	CPS6
ATOM	5366	CB	ILE	89	32.244	36.555	30.001	1.00 22.83	CPS6
ATOM	5367	CG2	ILE	89	33.564	36.820	30.736	1.00 22.49	CPS6
ATOM	5368	CG1	ILE	89	31.036	37.080	30.779	1.00 23.07	CPS6
ATOM	5369	CD1	ILE	89	30.876	36.460	32.168	1.00 23.21	CPS6
MOTA	5370	С	ILE	89	33.670	37.026	28.027	1.00 24.96	CPS6
MOTA	5371	0	ILE	89	33.990	35.997	27.435	1.00 24.10	CPS6
ATOM	5372	N	ILE	90	34.489	38.064	28.193	1.00 24.59	CPS6
ATOM	5373	CA	ILE	90	35.898	37.956	27.833	1.00 25.62	CPS6
MOTA	5374	CB	ILE	90	36.305	38.796	26.589	1.00 26.38	CPS6
ATOM	5375	CG2	ILE	90	35.630	38.229	25.360	1.00 26.74	CPS6
ATOM	5376	CG1	ILE	90	35.984	40.273	26.787	1.00 27.06	CPS6
ATOM	5377	CD1	ILE	90	36.410	41.147	25.584	1.00 30.06	CPS6
ATOM	5378	C	ILE	90	36.657	38.407	29.079	1.00 26.15	CPS6
ATOM	5379	0	ILE	90	36.241	39.337	29.783	1.00 25.40	CPS6
ATOM	5380	N	CYS	91	37.742	37.702	29.376	1.00 26.82	CPS6
ATOM	5381	CA	CYS	91	38.574	37.975	30.543	1.00 28.62	CPS6
ATOM	5382	CB	CYS	91	38.041	37.191	31.749	1.00 27.71	CPS6
MOTA	5383	SG	CYS	91	39.031	37.333	33.261	1.00 30.47	CPS6
ATOM	5384	С	CYS	91	39.998	37.516	30.194	1.00 29.98	CPS6
ATOM	5385	0	CYS	91	40.213	36.361	29.839	1.00 29.65	CPS6
ATOM	5386	N	THR	92	40.966	38.419	30.291	1.00 32.42	CPS6
MOTA	5387	CA	THR	92	42.344	38.078	29.948	1.00 34.14	CPS6
MOTA	5388	CB	THR	92	43.264	39.303	30.103	1.00 36.33	CPS6
ATOM	5389	OG1		92	43.150	39.810	31.439	1.00 38.35	CPS6
ATOM	5390		THR	92	42.872	40.393	29.104	1.00 35.90	CPS6
ATOM	5391	С	THR	92	42.931	36.932	30.761	1.00 35.10	CPS6
ATOM	5392	0	THR	92	43.960	36.359	30.380	1.00 36.58	CPS6
ATOM	5393	N	LYS	93	42.291	36.582	31.870	1.00 33.97	CPS6
ATOM	5394	CA	LYS	93	42.808	35.503	32.698	1.00 34.28	CPS6
ATOM	5395	CB	LYS	93	42.231	35.596	34.105	1.00 35.19	CPS6
ATOM	5396	CG	LYS	93	42.654	36.867	34.827	1.00 38.98	CPS6
ATOM	5397	CD	LYS	93	42.107	36.924	36.240	1.00 40.89	CPS6
ATOM	5398	CE	LYS	93	42.416	38.263	36.898	1.00 41.92	CPS6
ATOM	5399	NZ	LYS	93	43.879	38.529	36.966	1.00 43.76	CPS6
ATOM	5400	C	LYS	93	42.575	34.111	32.126	1.00 33.08	CPS6
ATOM	5401	0	LYS	93	43.143	33.137	32.613	1.00 33.58	CPS6
ATOM	5402	N	LEU	94	41.743	34.005	31.098	1.00 31.56	CPS6
ATOM	5403	CA	LEU	94	41.489	32.702	30.487	1.00 29.96	CPS6
ATOM	5404	CB	LEU	94	40.553	31.853	31.363	1.00 31.34	CPS6
ATOM	5405	CG	LEU	94	39.321	32.481	32.035	1.00 33.01	CPS6
ATOM	5406		LEU	94	38.520	33.306	31.062	1.00 32.91	CPS6
ATOM	5407		LEU	94	38.465	31.368	32.625	1.00 35.31	CPS6
ATOM	5408	C	LEU	94	40.917	32.822	29.091	1.00 28.50	CPS6
ATOM	5409	0	LEU	94	40.531	33.909	28.654	1.00 28.02	CPS6
ATOM	5410	N	SER	95	40.861	31.692	28.398	1.00 27.95	CPS6
ATOM	5411	CA	SER	95	40.341	31.636	27.040	1.00 27.87	CPS6
ATOM	5412	CB	SER	95	40.579	30.261	26.426	1.00 28.47	CPS6
ATOM	5413	OG	SER	95	39.846	30.141	25.218	1.00 30.54	CPS6
ATOM	5414	С	SER	95	38.849	31.905	27.011	1.00 26.60	CPS6



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FIG. 1A-95

TECH CENTER 1800/9900

	ATOM	5415	0	SER	95
	ATOM	5416	N	PRO	96
	ATOM	5417	CD	PRO	96
	ATOM	5418	CA	PRO	96
SS	ATOM	5419	CB	PRO	96
×	ATOM	5420	CG	PRO	96
. 5	ATOM	5421	C	PRO	96
의병	ATOM	5422	ō	PRO	96
U_ 10	ATOM	5423	N	ALA	97
4 8	ATOM	5424	CA	ALA	97
	ATOM	5425	CB	ALA	97
	ATOM	5426	c	ALA	97
APPROVED BY DRAFTSHAN	ATOM	5427	ō	ALA	97
13 E	ATOM	5428	N	ALA	98
ORAF	ATOM	5429	CA	ALA	98
4 6	ATOM	5430	CB	ALA	98
	ATOM	5431	C	ALA	98
	ATOM	5432	0	ALA	98
	ATOM	5432	И	VAL	98
	MOTA	5433		VAL	99
	ATOM	5434	CA CB	VAL	
	ATOM			VAL	99
		5436	CG1 CG2		99
	ATOM	5437		VAL	99
	ATOM	5438	C	VAL	99
	MOTA	5439	0	VAL	99
	ATOM	5440	N	HIS	100
	ATOM	5441	CA	HIS	100
	ATOM	5442	CB	HIS	100
	ATOM	5443	CG	HIS	100
	ATOM	5444	CD2	HIS	100
	ATOM	5445	ND1	HIS	100
	ATOM	5446	CE1	HIS	100
	ATOM	5447	NE2	HIS	100
	ATOM	5448	С	HIS	100
	ATOM	5449	0	HIS	100
	ATOM	5450	N	VAL	101
	ATOM	5451	CA	VAL	101
	ATOM	5452	CB	VAL	101
	ATOM	5453	CG1	VAL	101
	ATOM	5454	CG2	VAL	101
	ATOM	5455	С	VAL	101
	ATOM	5456	0	VAL	101
	ATOM	5457	N	SER	102
	ATOM	5458	CA	SER	102
	MOTA	5459	CB	SER	102
	ATOM	5460	OG	SER	102
	ATOM	5461	С	SER	102
	3 moss		_		

SER 102

ILE 103

ILE 103

ILE 103

ILE 103

ILE 103

THR 104

103

103

103

5462 O 5463 N

5464 CA 5465 CB

5469 C

5470 O

5471 N

5466 CG2 ILE

5467 CG1 ILE

5468 CD1 ILE

ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

MOTA

ATOM

ATOM

			TE	ECH CEN	TER 1600/2
38.098	31.331	27.793	1.00	25.68	CPS6
38.401	32.762	26.082	1.00	25.92	CPS6
39.206	33.567	25.144	1.00	25.77	CPS6
36.978	33.085	25.978	1.00	25.00	CPS6
36.947	34.199	24.922	1.00	25.69	CPS6
38.197	33.949	24.093	1.00	25.08	CPS6
36.129	31.873	25.602	1.00	25.28	CPS6
34.942	31.810	25.922	1.00	23.78	CPS6
36.741	30.902	24.934	1.00	24.13	CPS6
36.023	29.701	24.534	1.00	24.78	CPS6
36.873	28.890	23.569	1.00	25.54	CPS6
35.650	28.846	25.746	1.00	24.39	CPS6
34.783	27.980	25.657	1.00	25.77	CPS6
36.300	29.093	26.879	1.00	23.13	CPS6
36.033	28.320	28.094	1.00	23.12	CPS6
37.285	28.277	28.947	1.00	23.94	CPS6
34.875	28.867	28.937	1.00	23.29	CPS6
34.418	28.217	29.883	1.00	23.78	CPS6
34.398	30.055	28.593	1.00	22.50	CPS6
33.353	30.693	29.386	1.00	22.03	CPS6
33.776	32.130	29.747	1.00	22.74	CPS6
32.850	32.710	30.799	1.00	22.51	CPS6
35.207	32.132	30.250	1.00	24.89	CPS6
31.978	30.757	28.739	1.00	20.85	CPS6
31.850	30.969	27.534	1.00	20.38	CPS6
30.950	30.580	29.568	1.00	20.29	CPS6
29.563	30.652	29.132	1.00	18.65	CPS6
28.988	29.251	29.029	1.00	20.06	CPS6
29.786	28.360	28.139	1.00	23.66	CPS6
30.802	27.509	28.412	1.00	26.19	CPS6
29.626	28.343	26.772	1.00	25.30	CPS6
30.511	27.518	26.239	1.00	26.78	CPS6
31.237	27.000	27.214	1.00	27.25	CPS6
28.806	31.440	30.186	1.00	18.48	CPS6
29.071	31.297	31.378	1.00	17.96	CPS6
27.852	32.261	29.753	1.00	17.67	CPS6
27.092	33.060	30.697	1.00	17.87	CPS6
27.749	34.455	30.846	1.00	19.43	CPS6
27.766	35.151	29.492	1.00	19.75	CPS6
26.984	35.314	31.860	1.00	19.30	CPS6
25.650	33.255	30.229	1.00	17.14	CPS6
25.356	33.139	29.046	1.00	16.92	CPS6
24.752 23.365	33.522 33.821	31.173	1.00	17.82 18.24	CPS6
22.450	32.592	30.837	1.00	18.94	CPS6 CPS6
21.131	32.592	30.526	1.00	19.02	CPS6
22.932	34.853	31.855	1.00	17.95	CPS6
23.335	34.792	33.025	1.00	16.39	CPS6
22.112	35.802	31.414	1.00	16.51	CPS6
21.630	36.864	32.291	1.00	17.17	CPS6
22.243	38.240	31.884	1.00	17.60	CPS6
21.761	39.341	32.845	1.00	19.81	CPS6
23.769	38.152	31.899	1.00	19.89	CPS6
24.483	39.402	31.357	1.00	19.80	CPS6
20.112	36.933	32.131	1.00	17.69	CPS6
19.595	36.760	31.021	1.00	17.52	CPS6
19.414	37.173	33.237	1.00	18.18	CPS6
-2.214	3	33.237	1.00		50



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FIG. 1A-96

TECH CENTER 1600/2900

BY DLASS SUBCLASS

	MOTA	5472	CA	THR	104	17.954	37.283	33.226	1.00	18.92	CPS6
	MOTA	5473	CB	THR	104	17.285	35.948	33.660	1.00	20.47	CPS6
	MOTA	5474	OG1	THR	104	15.864	36.026	33.456	1.00	20.23	CPS6
	MOTA	5475	CG2	THR	104	17.578	35.648	35.130	1.00	17.86	CPS6
	ATOM	5476	С	THR	104	17.523	38.429	34.159	1.00	20.41	CPS6
	ATOM	5477	0	THR	104	18.306	38.901	34.990		19.19	CPS6
	ATOM	5478	N	HIS	105	16.280	38.880	34.001		21.31	CPS6
	ATOM	5479	CA	HIS	105	15.751	39.984	34.799		22.86	CPS6
	ATOM	5480	СВ	HIS	105	15.802	41.299	33.998		26.24	CPS6
	ATOM	5481	CG	HIS	105	17.175	41.721	33.578		30.59	CPS6
	ATOM	5482		HIS	105	17.889	41.444	32.461		32.14	CPS6
	ATOM	5483		HIS	105	17.974	42.534	34.355		33.04	CPS6
	ATOM	5484		HIS	105	19.122	42.739	33.733		33.19	CPS6
	ATOM	5485	NE2		105	19.097	42.089	32.582		32.49	CPS6
	ATOM	5486	C	HIS	105	14.278	39.762	35.129		23.27	
	ATOM	5487	ō	HIS	105	13.575	39.039	34.417		21.93	CPS6
	ATOM	5488	N	THR	106	13.837	40.393	36.212			
	ATOM	5489	CA	THR	106	12.430	40.333	36.605		23.40 25.56	CPS6
	ATOM	5490	CB	THR	106	12.430	39.537	37.816			CPS6
	ATOM	5491		THR	106					27.06	CPS6
	ATOM	5492		THR	106	12.664	40.059	39.015		26.80	CPS6
	MOTA	5493	C	THR	106		38.102	37.567		25.79	CPS6
	ATOM	5494	0	THR	106	12.266	41.879	37.013		27.51	CPS6
	ATOM	5495	N	LYS		13.230	42.651	36.964		26.39	CPS6
	MOTA	5496	CA	LYS	107	11.069	42.272	37.423		28.29	CPS6
	ATOM	5497	CB	LYS		10.880	43.662	37.810		29.88	CPS6
	ATOM	5498			107	9.440	43.899	38.268		32.33	CPS6
	ATOM	5498	CG	LYS	107	9.155	45.357	38.599		36.25	CPS6
			CD	LYS	107	7.745	45.549	39.147		39.84	CPS6
	MOTA MOTA	5500 5501	CE	LYS	107	7.473	47.024	39.442		41.42	CPS6
			NZ	LYS	107	6.102	47.246	39.995		45.05	CPS6
	ATOM	5502	C	LYS	107	11.839	44.132	38.905		29.50	CPS6
	MOTA	5503	0	LYS	107	12.367	45.243	38.823		29.28	CPS6
	MOTA	5504	N	GLU	108	12.081	43.289	39.912		27.21	CPS6
	MOTA	5505	CA	GLU	108	12.945	43.667	41.033		26.33	CPS6
	MOTA	5506	CB	GLU	108	12.239	43.363	42.358	1.00	30.27	CPS6
	MOTA	5507	CG	GLU	108	10.841	43.953	42.480		36.27	CPS6
	MOTA	5508	CD	GLU	108	10.259	43.782	43.874	1.00	41.02	CPS6
	ATOM	5509		GLU	108	10.158	42.632	44.354	1.00	44.74	CPS6
	MOTA	5510		GLU	108	9.897	44.803	44.497	1.00	45.09	CPS6
	MOTA	5511	C	GLU	108	14.333	43.033	41.108	1.00	25.31	CPS6
	NOM	5512	0	GLU	108	15.145	43.437	41.936	1.00	22.62	CPS6
	MOTA	5513	N	TYR	109	14.609	42.043	40.266	1.00	22.54	CPS6
	TOM	5514	CA	TYR	109	15.900	41.368	40.333	1.00	22.99	CPS6
	TOM	5515	CB	TYR	109	15.728	39.954	40.909	1.00	22.64	CPS6
	MOTA	5516	CG	TYR	109	15.175	39.906	42.310	1.00	24.37	CPS6
	MOTA	5517	CD1	TYR	109	15.988	40.167	43.411	1.00	24.51	CPS6
	MOTA	5518	CE1		109	15.465	40.190	44.701	1.00	26.40	CPS6
	MOTA	5519	CD2		109	13.821	39.661	42.531	1.00	24.67	CPS6
	MOTA	5520	CE2	TYR	109	13.286	39.683	43.809	1.00	24.88	CPS6
	MOTA	5521	cz	TYR	109	14.106	39.946	44.884	1.00	26.56	CPS6
	MOTA	5522	OH	TYR	109	13.576	39.968	46.144		29.07	CPS6
7	MOTA	5523	С	TYR	109	16.609	41.211	39.008		21.70	CPS6
2	MOTA	5524	0	TYR	109	15.993	41.280	37.945		22.54	CPS6
7	MOTA	5525	N	ALA	110	17.926	41.012	39.103		21.84	CPS6
Į	MOT	5526	CA	ALA	110	18.770	40.702	37.950		20.16	CPS6
7	TOM	5527	CB	ALA	110	19.785	41.803	37.666		21.73	CPS6
7	TOM	5528	С	ALA	110	19.492	39.445	38.443		20.44	CPS6
					-		-5.445	22.4.3			50



ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

5581 CA ARG 118

5582 CB ARG 118

5583 CG ARG 118

5584 CD ARG 118

5585 NE ARG 118

5529 0 ALA 110

5530 N ALA 111

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FIG. 1A-97

ATOM 5531 CA ALA 111 ATOM 5532 CB ALA 111 ATOM 5533 C ALA 111 ATOM 5534 0 ALA 111 CLASS SUBCLASS ATOM 5535 N 112 ALA ATOM 5536 CA 112 ALA ATOM 5537 CB ALA 112 ATOM 5538 С 112 ALA ATOM 5539 0 ALA 112 ATOM 5540 N GLN 113 5541 CA ATOM GLN 113 ATOM 5542 CB GLN 113 ATOM 5543 CG GLN 113 ATOM 5544 CD GLN 113 ATOM 5545 OE1 GLN 113 ATOM 5546 NE2 GLN 113 ATOM 5547 С GLN 113 ATOM 5548 0 GLN 113 И ATOM 5549 VAL 114 MOTA 5550 CA VAL 114 ATOM 5551 CB VAL 114 ATOM 5552 CG1 VAL 114 ATOM 5553 CG2 VAL 114 ATOM 5554 C VAL 114 ATOM 5555 0 VAL 114 5556 ATOM N VAL 115 ATOM 5557 CA VAL 115 ATOM 5558 CB VAL 115 ATOM 5559 CG1 VAL 115 ATOM 5560 CG2 VAL 115 ATOM 5561 С VAL 115 ATOM 5562 О VAL 115 ATOM 5563 N ILE 116 ATOM 5564 CA ILE 116 ATOM 5565 CB ILE 116 ATOM 5566 CG2 ILE 116 ATOM 5567 CG1 ILE 116 ATOM 5568 CD1 ILE 116 ATOM 5569 C ILE 116 ATOM 5570 0 ILE 116 ATOM 5571 N GLU 117 ATOM 5572 CA GLU 117 ATOM 5573 CB GLU 117 ATOM 5574 CG GLU 117 ATOM 5575 CD GLU 117 ATOM 5576 OE1 GLU 117 ATOM 5577 OE2 GLU 117 ATOM 5578 GLU 117 ATOM 5579 0 GLU 117 ATOM 5580 N ARG

118

38.479

19.996

34.930

1.00 50.78

CPS6

19.824	39.345	39.621	1.00 21.38	CPS6
19.714	38.476	37.560	1.00 19.56	CPS6
20.415	37.272	37.962	1.00 17.92	CPS6
19.410	36.180	38.358	1.00 18.78	CPS6
21.286	36.791	36.808	1.00 18.10	CPS6
21.044	37.114	35.654	1.00 19.16	CPS6
22.319	36.033	37.128	1.00 18.13	CPS6
23.175	35.509	36.083	1.00 18.42	CPS6
24.206	36.565	35,659	1.00 16.42	CPS 6
23.882	34.260	36.569	1.00 17.57	CPS6
24.000	34.017	37.778	1.00 18.87	CPS6
24.327	33.449	35.619	1.00 17.13	CPS6
25.065 24.163	32.247	35.971	1.00 17.77	CPS6
23.699	31.017 30.693	35.898	1.00 19.54	CPS6
22.787	29.472	34.495 34.435	1.00 21.95	CPS6
22.446	29.002	33.352	1.00 25.73 1.00 27.72	CPS6
22.378	28.968	35.594	1.00 27.72	CPS6 CPS6
26.205	32.133	34.968	1.00 16.69	CPS6
26.104	32.622	33.840	1.00 16.20	CPS6
27.288	31.499	35.391	1.00 17.22	CPS6
28.449	31.324	34.535	1.00 17.47	CPS6
29.605	32.300	34.948	1.00 17.72	CPS6
30.931	31.901	34.243	1.00 16.56	CPS6
29.222	33.738	34.581	1.00 17.27	CPS6
28.964	29.911	34.693	1.00 18.72	CPS6
28.880	29.338	35.776	1.00 19.21	CPS6
29.461	29.338	33.604	1.00 18.94	CPS6
30.090	28.027	33.684	1.00 19.93	CPS6
29.311	26.916	32.928	1.00 19.40	CPS6
30.143 27.981	25.631	32.901	1.00 20.42	CPS6
31.453	26.638	33,628	1.00 19.61	CPS6
31.453	28.231 28.860	33.023 31.958	1.00 20.14 1.00 19.69	CPS6
32.498	27.750	33.680	1.00 19.69	CPS6 CPS6
33.839	27.853	33.121	1.00 19.47	CPS6
34.806	28.617	34.068	1.00 21.42	CPS6
36.235	28.577	33.505	1.00 23.06	CPS6
34.365	30.082	34.195	1.00 21.71	CPS6
35.180	30.906	35.213	1.00 21.07	CPS6
34.320	26.420	32.940	1.00 24.10	CPS6
34.264	25.615	33.872	1.00 23.26	CPS6
34.759	26.103	31.731	1.00 25.26	CPS6
35.243	24.769	31.424	1.00 29.11	CPS6
34.878	24.369	30.001	1.00 30.47	CPS6
33.446	24.548	29.587	1.00 33.45	CPS6
33.226	24.007	28.194	1.00 36.82	CPS6
33.345	22.776	28.022	1.00 39.37	CPS6
32.959	24.804	27.271	1.00 38.14	CPS6
36.754	24.698	31.503	1.00 31.19	CPS6
37.445 37.259	25.712	31.392	1.00 28.72	CPS6
37.259	23.484	31.686 31.686	1.00 34.06 1.00 39.18	CPS6
39.089	22.180	32.703	1.00 39.18	CPS6 CPS6
38.327	20.872	32.703	1.00 46.37	CPS6
38.840	19.776	33.528	1.00 49.12	CPS6
		23.320		22.50



SEP 0 9 2002

FIG. 1A-98

FIG.	SUBCLASS	
0.6. F	OLASS	
AT PROVED	ξŝ	BAFTSMAN

ATOM	5586	CZ	ARG	118	39.095	20.849	35.744	1.00 51.80	CPS6
ATOM	5587	NH1	ARG	118	40.113	21.575	35.304	1.00 53.03	CPS6
ATOM	5588	NH2	ARG	118	38.692	20.977	37.003	1.00 51.56	CPS6
ATOM	5589	С	ARG	118	38.895	22.789	30.250	1.00 40.50	CPS6
ATOM	5590	0	ARG	118	38.365	21.750	29.862	1.00 41.56	CPS6
ATOM	5591	N	LEU	119	39.615	23.562	29.445	1.00 42.65	CPS6
ATOM	5592	CA	LEU	119	39.833	23.176	28.055	1.00 44.91	CPS6
ATOM	5593	CB	LEU	119	40.106	24.414	27.196	1.00 45.15	CPS6
ATOM	5594	CG	LEU	119	38.970	25.432	27.070	1.00 45.37	CPS6
ATOM	5595		LEU	119	39.442	26.618	26.246	1.00 44.17	CPS6
ATOM	5596		LEU	119	37.752	24.776	26.427	1.00 45.02	CPS6
			LEU	119	40.991	22.193	27.918	1.00 45.02	CPS6
ATOM	5597	C	LEU	119	41.823	22.133	28.848	1.00 47.25	CPS6
ATOM	5598	OT2		119	41.055	21.501	26.874	1.00 47.76	CPS6
ATOM	5599				74.183		-19.320	1.00 47.76	AT
MOTA	5600	0	HOH	1				1.00 16.24	AT
ATOM	5601	0	HOH	2	50.451	28.498	2.245		
MOTA	5602	0	нон	3	72.513	43.845	5.247	1.00 16.95	AT
ATOM	5603	0	нон	4	59.768	49.591	13.381	1.00 18.99	AT
MOTA	5604	0	HOH	5	9.919	40.963	40.359	1.00 17.22	AT
ATOM	5605	0	HOH	6	57.301	49.721	15.536	1.00 18.51	AT
MOTA	5606	0	HOH	7	72.254	36.424	22.184	1.00 19.44	TA
MOTA	5607	0	HOH	8	15.486	40.288	48.189	1.00 19.00	AT
MOTA	5608	0	HOH	9	22.359	26.422	33.132	1.00 28.69	AΤ
MOTA	5609	0,	HOH	10	62.648	41.000	12.765	1.00 26.69	AT
ATOM	5610	0	HOH	11	27.253	11.532	60.836	1.00 33.03	AT
ATOM	5611	0	HOH	12	4.545	29.482	16.753	1.00 34.49	AT
ATOM	5612	0	HOH	13	14.678	33.346	17.568	1.00 28.16	AT
ATOM	5613	0	HOH	14	2.443	17.966	21.642	1.00 31.50	AT
ATOM	5614	0	HOH	15	13.387	44.897	46.109	1.00 36.84	AT
ATOM	5615	0	HOH	16	64.048	43.971	9.189	1.00 27.36	AΤ
ATOM	5616	0	HOH	17	17.153	29.081	61.693	1.00 38.80	AT
MOTA	5617	0	HOH	18	15.565	11.097	37.041	1.00 32.04	AT
ATOM	5618	0	HOH	19	66.736	39.802	9.758	1.00 31.88	AT
ATOM	5619	0	HOH	20	68.806	35.163	19.609	1.00 43.12	AT
ATOM	5620	0	HOH	21	28.442	30.448	25.270	1.00 35.30	AT
ATOM	5621	0	HOH	22	20.356	37.769	28.103	1.00 40.41	AT
ATOM	5622	0	HOH	23	27.784	56.284	42.007	1.00 39.44	AT
ATOM	5623	0	HOH	24	9.819	21.853	51.711	1.00 48.93	AT
ATOM	5624	ō	нон	25	18.794	48.571	49,608	1.00 38.44	AT
ATOM	5625	ŏ	нон	26	50.953	43.970	28.198	1.00 29.58	AT
ATOM	5626	ō	нон	27	22.120	28.021	18.001	1.00 41.70	AT
ATOM	5627	ō	нон	28	18.224	7.825	50.971	1.00 37.65	AT
ATOM	5628	Ö	нон	29	45.010	40.785	1.909	1.00 35.18	AT
ATOM	5629	ō	нон	30	64.211	31.229	23.988	1.00 42.82	AT
ATOM	5630	ŏ	нон	31	55.673	59.846	2.934	1.00 40.75	AT
ATOM	5631	0	HOH	32	12.144	16.656	71.990	1.00 45.41	AT
ATOM	5632	0	HOH				35.889	1.00 33.23	AT
ATOM	5633	0		33	26.174	28.070		1.00 33.23	AT
			HOH	34	23.423	24.108	37.385		
MOTA	5634	0	нон	35	72.206	58.375	9.452	1.00 45.41	AT
ATOM	5635	0	HOH	36	4.583	28.820	43.211	1.00 37.91	AT
ATOM	5636	0	нон	37	54.428	31.469	26.691	1.00 40.61	AT
ATOM	5637	0	нон	38	5.129	39.360	42.159	1.00 34.31	AT
ATOM	5638	0	HOH	39	61.288	9.543	3.422	1.00 45.78	AT
MOTA	5639	0	HOH	40	41.144	21.554	50.056	1.00 46.77	AT
MOTA	5640	0	нон	41	45.899	31.375	23.218	1.00 36.69	AT
MOTA	5641	0	нон	42	46.684	40.019	4.072	1.00 40.88	AT
MOTA	5642	0	HOH	43	32.060	30.436	24.972	1.00 38.00	AT



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SERAGO



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BY CLASS SUBCLASS

FIG. 1A-99

MOTA	5643	0	HOH	44	27.193	55.260	39.276	1.00 39.83	AT
ATOM	5644	0	HOH	45	74.083	12.016	10.419	1.00 37.57	AT
MOTA	5645	0	HOH	46	7.161	11.806	20.918	1.00 37.74	AΤ
ATOM	5646	0	HOH	47	37.597	37.224	10.717	1.00 44.06	AT
ATOM	5647	0	HOH	48	26.713	40.428	46.123	1.00 47.01	AT
ATOM	5648	0	HOH	49	73.327	31.524	18.039	1.00 39.95	TA
ATOM	5649	0	HOH	50	6.885	35.701	48.910	1.00 38.11	AT
ATOM	5650	0	HOH	51	12.147	30.555	62.867	1.00 45.67	AT
ATOM	5651	0	HOH	52	45.035	35.126	28.209	1.00 45.09	AT
ATOM	5652	0	HOH	53	45.816	30.463	0.531	1.00 37.06	AT
MOTA	5653	0	HOH	54	37.959	49.546	12.787	1.00 41.97	AT
ATOM	5654	0	HOH	55	29.307	59.252	40.586	1.00 54.29	AT
ATOM	5655	0	HOH	56	33.064	30.245	14.482	1.00 53.18	ΑT
ATOM	5656	0	HOH	57	5.959	29.404	40.923	1.00 42.88	AT
ATOM	5657	0	HOH	58	72.015	56.594	2.111	1.00 41.98	AT
MOTA	5658	0	HOH	59	34.149	9.199	46.267	1.00 42.25	AT
MOTA	5659	0	HOH	60	56.871	24.901	5.890	1.00 43.48	AT
ATOM	5660	0	HOH	61	53.366	27.278	27.533	1.00 46.43	TA
ATOM	5661	0	HOH	62	51.684	37.046	30.830	1.00 46.25	TA
ATOM	5662	0	HOH	63	52.569	48.531	8.124	1.00 42.45	AT
MOTA	5663	0	HOH	64	19.990	15.518	32.236	1.00 48.76	AT
MOTA	5664	0	HOH	65	64.540	44.979	26.386	1.00 42.49	AT
MOTA	5665	0	HOH	66	30.220	13.054	46.228	1.00 52.13	TA
MOTA	5666	0	HOH	67	54.239	52.985	1.438	1.00 45.12	TA
MOTA	5667	0	HOH	68	20.023	54.748	37.127	1.00 39.76	TA
MOTA	5668	0	HOH	69	8.456	21.336	37.515	1.00 48.76	TA
ATOM	5669	0	HOH	70	35.909	45.522	2.599	1.00 46.39	AT
ATOM	5670	0	HOH	71	53.886	30.997	19.731	1.00 43.92	AT
ATOM	5671	0	HOH	72	10.033	24.488	66.210	1.00 53.66	AT
ATOM	5672	0	HOH	73	58.903	57.250	13.037	1.00 41.23	AT
ATOM	5673	0	HOH	74	62.777	15.875	1.984	1.00 41.20	AT
ATOM	5674	0	HOH	75	42.217	40.323	33.742	1.00 43.11	AT
ATOM	5675	0	HOH	76	20.956	40.692	29.179	1.00 49.81	AT
ATOM	5676	0	HOH	77	46.166	43.977	11.730	1.00 36.26	AT
ATOM	5677	0	HOH	78	66.744	59.058	16.145	1.00 56.18	AT
ATOM	5678	0	HOH	79	45.851	25.881	4.391	1.00 55.88	AT
ATOM	5679	0	HOH	80	75.174	49.183	6.063	1.00 47.74	AT
ATOM	5680	0	HOH	81	29.310	41.802	17.220	1.00 55.92	AT
ATOM	5681	0	HOH	82	1.927	35.649	42.778	1.00 51.25	AT
ATOM	5682	0	HOH	83	-1.663	38.805	38.155	1.00 39.95	AT
ATOM	5683	0	HOH	84	14.052	11.606	52.410	1.00 45.64	AT
MOTA	5684	0	HOH	85	12.374	37.222	15.756	1.00 49.24	AT
ATOM	5685	0	нон	86	31.903	41.930	45.468	1.00 45.19	AT
ATOM	5686	0	нон	87	33.483	20.380	56.292	1.00 53.83	AT
ATOM	5687	0	HOH	88	74.639	45.461	5.020	1.00 41.59	AT
ATOM	5688	0	HOH	89	37.028	19.108	53.278	1.00 43.77	AT
ATOM	5689	0	HOH	90	38.593	49.011	6.342	1.00 51.49	AT
MOTA	5690	0	HOH	91	52.402	56.617	3.593	1.00 53.57	AT
ATOM	5691	o	нон	92	5.772	28.675	61.930	1.00 44.14	AT
ATOM	5692	ō	нон	93	32.173	36.302	19.628	1.00 45.70	AT
ATOM	5693	0	HOH	94	52.026	42.123	29.953	1.00 47.73	AT
ATOM	5694	o	нон	95	47.042	40.027	29.849	1.00 57.66	AT
ATOM	5695	0	HOH	96	62.041	43.614	30.370	1.00 49.31	AT
ATOM	5696	0	нон	97	61.630	30.997	18.476	1.00 53.79	AT
ATOM	5697	ō	HOH	98	11.168	13.661	45.409	1.00 45.46	AT

28.738 15.678 20.064 1.00 63.95

37.162 57.858 42.839 1.00 49.29

AT

AT

5698 O

ATOM 5699 0

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HOH 100



SEP 0 9 2002

TECH CENTER 1600/2900

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MOTA	5700	0	HOH	101	56.970	48.398	18.183	1.00	20.07	AT
MOTA	5701	0	HOH	102	16.747	17.196	32.059	1.00	21.58	AT
ATOM	5702	0	HOH	103	45.835	52.603	17.631	1.00	19.92	AT
ATOM	5703	o	нон	104	-5.526	20.298	17.919	1.00	20.40	TA
MOTA	5704	ō	нон	105	16.573	18.225	29.320		21.11	AT
ATOM	5705	ō	нон	106	28.084	33.122	26.572		21.96	AT
ATOM	5706	ŏ	нон	107	56.776	49.897	20.691		20.77	AT
		0	нон	108	61.822	31.586	15.608			
ATOM	5707	-							22.44	AT
MOTA	5708	0	нон	109	75.499	25.254	21.262		22.49	AT
ATOM	5709	0	нон	110	52.716	36.178	-8.615		23.96	AT
ATOM	5710	0	нон	111	30.657	33.717	27.675		22.13	AT
ATOM	5711	0	HOH	112	31.857	23.322	43.883		22.91	AT
ATOM	5712	0	нон	113	16.560	16.176	27.250	1.00	22.50	TA
MOTA	5713	0	HOH	114	48.919	55.521	18.754	1.00	22.71	AT
MOTA	5714	0	HOH	115	30.469	45.806	26.160	1.00	24.06	AT
MOTA	5715	0	HOH	116	29.611	29.912	44.889	1.00	23.26	AT
MOTA	5716	0	HOH	117	14.658	45.605	43.596	1.00	25.77	AT
ATOM	5717	0	HOH	118	38.482	35.704	27.602	1.00	23.84	TA
ATOM	5718	0	нон	119	33.048	33.856	26.010		23.17	TA
ATOM	5719	ō	нон	120	11.956	35.757	52.609		26.32	ΑT
ATOM	5720	0	нон	121	72.585	45.998	2.976		23.39	AT
ATOM	5721	ō	нон	122	45.040	32.707	1.982		25.55	TA
ATOM	5722	o	нон	123	71.609	48.727	2.944		24.67	AT
ATOM	5723									
		0	HOH	124	34.369	7.558	43.913		24.87	AT
ATOM	5724	0	нон	125	4.595	36.818	41.429		25.98	AT
ATOM	5725	0	нон	126	11.206	23.871	43.608		25.23	TA
MOTA	5726	0	HOH	127	14.284	14.636	65.129		25.02	TA
MOTA	5727	0	HOH	128	70.983	32.077	16.439		25.53	TA
ATOM	5728	0	HOH	129	15.935	10.066	59.658	1.00	25.84	ΑT
MOTA	5729	0	HOH	130	17.042	11.420	57.203	1.00	25.22	TA
ATOM	5730	0	HOH	131	78.508	30.572	16.070	1.00	25.80	AΤ
MOTA	5731	0	HOH	132	31.882	25.438	41.276	1.00	25.44	TA
ATOM	5732	0	HOH	133	68.333	21.576	13.174	1.00	27.25	AT
ATOM	5733	0	HOH	134	59.808	51.543	15.137	1.00	26.71	AT
MOTA	5734	0	нон	135	51.803	45.823	2.829		28.23	AT
MOTA	5735	0	нон	136	23.948	33.437	19.543		26.93	AT
ATOM	5736	0	нон	137	77.529	24.686	-0.187		27.06	AT
ATOM	5737	ō	нон	138	36.414	47.961	27.068		26.59	AT
ATOM	5738	o	нон	139	15.210	37.727	30.916		26.63	AT
ATOM	5739	o	нон	140						
ATOM	5740		нон		26.736	13.803	59.642		27.51	AT
ATOM		0		141	59.707	29.029	-5.923		28.00	AT
	5741	0	нон	142	73.385	50.907	2.916		25.70	AT
MOTA	5742	0	HOH	143	25.372	31.413	54.764		28.23	AT
ATOM	5743	0	нон	144	8.726	40.753	36.473		28.04	AT
ATOM	5744	0	HOH	145	21.631	52.226	39.835	1.00	27.68	AT
MOTA	5745	0	HOH	146	6.966	31.512	19.584	1.00	26.22	AT
ATOM	5746	0	HOH	147	33.568	23.343	41.390	1.00	28.59	AT
ATOM	5747	0	HOH	148	47.104	33.497	24.474	1.00	31.57	AT
MOTA	5748	0	HOH	149	42.706	46.788	25.123	1.00	28.27	AT
ATOM	5749	0	HOH	150	15.361	13.776	53.744	1.00	28.43	AT
ATOM	5750	0	нон	151	49.210	27.704	6.023		26.48	AT
ATOM	5751	0	нон	152	69.742	37.893	23.208		28.63	AT
ATOM	5752	0	нон	153	62.896	46.941	28.207		29.51	AT
ATOM	5753	ō	нон	154	66.194	34.304	-2.754		27.04	AT
ATOM	5754	ō	нон	155	56.380	56.783	12.351		29.49	AT
ATOM	5755	ŏ	нон	156	62.810	23.721	9.697		29.08	AT
ATOM	5756	ŏ	нон	157			-20.735		30.39	AT
	2.33	-	.1011	137	59.600	48.626	-20.735	1.00	30.39	A1

FIG. 1A-100



SEP 0 9 2002



TECH CENTER 1600/2900 FIG. 1A-101

: IG.	SUBCLASS	
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ATOM	5757	0	HOH	158	63.447	33.873	17.572	1.00 29.71	AT
ATOM	5758	0	HOH	159	11.724	13.599	66.211	1.00 27.82	AT
ATOM	5759	0	HOH	160	60.558	22.006	10.718	1.00 28.85	AT
ATOM	5760	0	HOH	161	46.499	54.700	19.899	1.00 29.19	AT
ATOM	5761	0	HOH	162	63.410	57.441	-12.830	1.00 29.14	AT
ATOM	5762	0	HOH	163	16.531	13.383	27.915	1.00 29.15	AT
ATOM	5763	0	HOH	164	57.094	58.123	-5.057	1.00 30.67	AT
ATOM	5764	0	HOH	165	55.029	24.601	-1.884	1.00 27.07	AT
ATOM	5765	0	HOH	166	13.338	35.151	24.133	1.00 28.54	AT
ATOM	5766	0	HOH	167	35.398	47.783	6.493	1.00 28.26	AT
ATOM	5767	0	HOH	168	70.174	56.885	-10.515	1.00 31.78	AT
ATOM	5768	0	HOH	169	25.901	44.946	25.667	1.00 31.94	AT
ATOM	5769	0	HOH	170	50.393	53.846	23.119	1.00 28.26	AT
ATOM	5770	0	HOH	171	62.156	25.716	13.450	1.00 31.00	AT
ATOM	5771	0	HOH	172	42.474	44.185	26.823	1.00 31.95	AT
ATOM	5772	0	HOH	173	77.820	49.020	-5.810	1.00 32.32	AT
ATOM	5773	0	HOH	174	67.420		-19.340	1.00 29.68	AT
ATOM	5774	0	HOH	175	48.791	40.644	-3.702	1.00 28.90	AT
ATOM	5775	0	HOH	176	33.117	16.234	43.002	1.00 31.48	AT
ATOM	5776	0	HOH	177	15.122	24.092	63.819	1.00 30.47	AT
ATOM	5777	0	HOH	178	64.991	30.299	-1.464	1.00 30.76	AT
ATOM	5778	0	HOH	179	15.212	16.862	21.098	1.00 32.61	AT
ATOM	5779	0	HOH	180	8.026	30.440	48.746	1.00 29.36	AT
ATOM	5780	0	HOH	181	15.063	29.611	60.193	1.00 29.52	AT
ATOM	5781	0	нон	182	-4.236	31.973	27.775	1.00 33.07	AT
ATOM	5782	0	HOH	183	41.379	28.581	29.607	1.00 31.08	AT
ATOM	5783	0	HOH	184	30.685	20.525	44.633	1.00 30.33	AT
ATOM	5784	0	HOH	185	25.786	35.845	47.678	1.00 31.51	AT
ATOM	5785	0	HOH	186	33.235	47.941	17.895	1.00 29.68	AT
ATOM	5786	0	HOH	187	64.882	30.921	17.515	1.00 30.10	AT
ATOM	5787	0	HOH	188	5.685	13.963	30.264	1.00 32.30	AT
ATOM	5788	0	HOH	189	-4.735	20.413	39.978	1.00 33.19	AT
ATOM	5789	0	нон	190	44.587	45.272	8.578	1.00 31.21	AT
ATOM	5790	0	нон	191	57.838	12.743	11.965	1.00 31.21	AT
ATOM	5791	0	нон	192	16.393	22.844	66.100	1.00 34.23	AT
ATOM	5792	0	HOH	193	4.372	22.943	37.792	1.00 32.96	AT
ATOM	5793	0	HOH	194	71.929	20.305	14.473	1.00 32.09	AT
ATOM	5794	0	HOH	195	28.925	15.553	59.281	1.00 30.49	AT
ATOM	5795	0	HOH	196	53.796	25.895	-4.052	1.00 33.01	AT
ATOM	5796	0	HOH	197	6.468	23.780	36.296	1.00 34.02	AT
ATOM	5797	0	HOH	198	53.710	44.972	-1.506	1.00 33.84	AT
ATOM	5798	0	HOH	199	19.319	42.034	48.498	1.00 31.81	AT
ATOM	5799	0	нон	200	24.603	12.893	57.779	1.00 32.45	AT
ATOM	5800	0	HOH	201	82.186	45.693	-2.681	1.00 34.17	AT
ATOM	5801	0	нон	202	11.264	18.716	60.799	1.00 36.53	AT
ATOM	5802	0	нон	203	79.085	17.668	9.255	1.00 30.53	AT
ATOM	5803	0	HOH	204	59.866	52.931	11.834	1.00 30.91	AT
ATOM	5804	0	нон	205	13.907	16.278	62.855	1.00 36.18	AT
ATOM	5805	0	нон	206	16.412	14.129	56.660	1.00 30.18	AT
ATOM	5806	0	нон	207	66.234	40.890	-9.847	1.00 32.42	
ATOM	5807	ō	нон	208	10.481	11.237	25.068	1.00 31.86	AT AT
ATOM	5808	ō	нон	209	5.289	19.707	30.585	1.00 32.03	AT
ATOM	5809	ō	нон	210	39.446	40.017	23.668	1.00 33.17	
ATOM	5810	ō	нон	211	54.509	23.461		1.00 35.31	AT
ATOM	5811	ō	нон	212	51.401	31.567	6.035	1.00 35.31	AT AT
ATOM	5812	ō	нон	213	28.205	23.736	11.354	1.00 32.75	AT
ATOM	5813	ō	нон	214	50.324		55.152		
·		-			30.324	34.946	-7.659	1.00 34.98	AT



SEP 0 9 2002 **TECH CENTER 1600/2900**

FIG. 1A-102



ATOM	5814	0	HOH	215	30.129	20.719	56.661	1.00 32.37	AT
ATOM	5815	0	HOH	216	58.457	50.516	-18.849	1.00 32.27	AT
ATOM	5816	0	HOH	217	44.476	34.908	24.562	1.00 35.00	AT
ATOM	5817	0	HOH	218	9.990	35.69 3	24.724	1.00 34.96	AT
ATOM	5818	0	HOH	219	11.096	35.811	32.093	1.00 34.27	AT
ATOM	5819	0	HOH	220	12.913	17.730	46.309	1.00 34.71	AT
ATOM	5820	o	HOH	221	65.231	44.053	-7.852	1.00 32.99	AT
ATOM	5821	o	HOH	222	38.789	35.275	9.625	1.00 34.60	AT
MOTA	5822	o	нон	223	12.929	25.623	47.543	1.00 32.40	AT
ATOM	5823	ō	нон	224	74.529	33.737	18.589	1.00 33.85	AT
ATOM	5824	ō	нон	225	16.279	43.522	36.165	1.00 33.82	AT
ATOM	5825	ō	HOH	226	13.480	14.423	55.667	1.00 35.36	AT
ATOM	5826	ŏ	нон	227	4.656	17.272	27.720	1.00 34.90	AT
ATOM	5827	ō	нон	228	55.566	43.939		1.00 37.00	AT
ATOM	5828	o	нон	229	18.454	21.396	68.984	1.00 37.00	TA
MOTA	5829	ō	нон	230	56.014	51.348		1.00 37.91	AT
ATOM	5830	ō	HOH	231	71.572	46.002	-9.177	1.00 36.91	AT
ATOM	5831	ŏ	HOH	232	39.465	30.116	20.475	1.00 46.92	AT
ATOM	5832	ō	HOH	233	40.113	37.155	25.795	1.00 31.64	TA
ATOM	5833	ő	нон	234	14.226	44.782	35.447	1.00 33.52	AT
ATOM	5834	ő	нон	235	20.027	45.208	30.512	1.00 33.32	AT
ATOM	5835	ŏ	HOH	236	61.895	17.484	0.210	1.00 36.39	AT
ATOM	5836	ŏ	HOH	237	26.769	18.525	65.425	1.00 38.39	AT
ATOM	5837	ō	HOH	238	30.216	49.429	23.557	1.00 38.87	AT
ATOM	5838	ŏ	HOH	239	12.005	18.680	49.514	1.00 35.80	AT
ATOM	5839	o	нон	240	40.174	39.987	26.354	1.00 35.80	AT
ATOM	5840	ő	нон	241	19.654	14.821	28.728	1.00 35.91	AT
ATOM	5841	ŏ	нон	242	55.447	29.046	11.959	1.00 35.91	AT
ATOM	5842	ŏ	HOH	243	67.323	29.753	-3.238	1.00 39.47	AT
ATOM	5843	ŏ	нон	244	84.687	32.541	17.389	1.00 39.50	AT
ATOM	5844	ŏ	HOH	245	54.503	28.663	-6.976	1.00 36.28	AT
ATOM	5845	ō	нон	246	35.636	37.561	8.625	1.00 35.25	AT
ATOM	5846	ō	нон	247	10.020	25.331	46.396	1.00 38.25	AT
ATOM	5847	ō	нон	248	11.151	27.733	14.203	1.00 38.25	AT
ATOM	5848	ō	HOH	249	10.978	20.075	53.913	1.00 38.20	
ATOM	5849	ŏ	HOH	250	77.340	21.792			AT
ATOM	5850	ŏ	нон	251	63.681	23.994	0.783	1.00 40.63	AT
ATOM	5851	ŏ	HOH	252	11.477	23.994	15.360	1.00 37.38	AT
ATOM	5852	o	нон	253			48.380	1.00 37.57	AT
ATOM	5853	o	HOH	254	24.484	40.133	44.556	1.00 37.00	AT
ATOM	5854	0	HOH	255	26.870 38.821	34.997	63.642	1.00 37.28	AT
ATOM	5855	0	HOH	256	17.119	41.107	28.862	1.00 37.55	AT
ATOM	5856	o	нон	257		53.559	27.111	1.00 35.75	AT
ATOM	5857	ŏ	нон	258	31.732	49.464	21.724	1.00 40.71	AT
ATOM	5858	ŏ	HOH	259	37.233	48.595	24.778	1.00 37.38	AT
ATOM	5859	ō	нон	260	64.957	31.599	-4.165	1.00 34.72	AT
ATOM	5860	0	HOH	261	42.059	35.767	26.985	1.00 38.69	AT
ATOM	5861	ŏ	нон	262	53.170	52.497	-1.737	1.00 41.39	AT
ATOM	5862	o	HOH		15.919	8.802	51.909	1.00 37.27	AT
ATOM	5863	0	HOH	263	60.591	34.941	-9.345	1.00 36.16	AT
ATOM	5864	0		264	10.541	36.936	29.724	1.00 38.71	AT
ATOM	5865	0	HOH	265	31.514	44.281	21.202	1.00 36.97	AT
ATOM	5866	0	HOH	266	9.564	36.687	51.380	1.00 38.68	ΑT
ATOM	5867	0		267	79.927	33.538	17.348	1.00 38.09	AT
ATOM	5868	0	HOH HOH	268	52.604	28.637	11.241	1.00 38.37	AT
ATOM	5869	0		269	4.383	30.021	19.676	1.00 37.95	AT
ATOM	5870	0	НОН НОН	270	39.831	37.961	44.275	1.00 39.26	AT
21.00	3070	J	nOH	271	76.908	49.901	-8.433	1.00 40.20	ΑT



ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

5920 O HOH 321

5921 0 нон 322

5922 0 HOH 323

5923 O HOH 324

5924 O HOH 325

5925 0 HOH 326

5926 0 нон 327

5927 0 HOH 328

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FIG. 1A-103

ATOM 5871 Ω HOH 272 18.828 14.845 36.392 1.00 40.61 AΤ ATOM 5872 0 HOH 273 77.377 18 239 12 575 1.00 39.42 AΤ ATOM 13.536 5873 0 нон 274 51.042 29.821 1.00 39.59 AT ATOM 5874 0 нон 275 64.107 14.629 14.266 1.00 39.71 AΤ ATOM 5875 0 HOH 276 58.267 58.162 -7.799 1.00 39.43 AΤ ATOM 5876 0 HOH 277 40.740 40.966 31.483 1.00 40.51 AT ATOM 5877 0 нон 278 15.055 10.589 55.645 1.00 39.15 AT ATOM 5878 0 HOH 279 19.789 34.347 51.860 1.00 40.37 AΤ ATOM 5879 0 HOH 280 11.976 38.727 31.710 1.00 37.91 AT ATOM 5880 0 HOH 281 31.389 28.117 42 824 1.00 40.91 AT ATOM 5881 0 нон 282 70.878 25.270 -4.197 1.00 43.53 AT ATOM 5882 0 нон 283 75.431 41.776 4.726 1.00 40.67 AT ATOM 5883 0 HOH 284 62.312 53.358 28.086 1.00 40.98 ΑT ATOM 5884 0 нон 285 62.124 59.105 9.640 1.00 39.55 AТ ATOM 5885 0 нон 286 40.707 28.142 23.532 1.00 44.54 AT ATOM 5886 0 нон 287 33.311 41.660 3.153 1.00 41.98 AT ATOM 5887 0 HOH 288 38.680 48,495 32.258 1.00 44.14 AT MOTA 5888 0 нон 289 32.712 38.251 44.880 1.00 40.32 AT ATOM 5889 0 нон 290 12.709 24.006 64.828 1.00 40.21 AT ATOM 5890 O нон 291 48.861 28.304 14.453 1.00 42.61 AT ATOM 5891 0 HOH 292 79.466 20.245 8.333 1.00 40.49 ΑT ATOM 5892 0 HOH 293 50.553 45.041 -0.292 1.00 42.19 ΔТ ATOM 5893 0 нон 42.897 294 26.326 5.722 1.00 41.10 AT ATOM 5894 0 HOH 295 40.124 38.889 3.911 1.00 42.97 ΑT -9.725 ATOM 5895 0 нон 296 26.259 40.147 1.00 43.57 AT ATOM 5896 0 нон 24.463 297 39.296 47.536 1.00 39.76 AT ATOM 5897 0 HOH 298 59.389 43.519 -22.049 1.00 45.90 AT ATOM 5898 0 нон 299 58.697 26.078 -8.432 1.00 42.64 AT ATOM 5899 0 HOH 300 59.168 23.233 -8.586 1.00 43.13 ΑT ATOM 5900 0 нон 301 33.173 10.853 42.976 1.00 43.47 AT ATOM 5901 0 нон 302 38.135 51.041 21.685 1.00 40.23 AT ATOM 5902 O HOH 303 64.003 32.204 20.781 1.00 39.51 ΑT MOTA 5903 0 HOH 304 18.175 36.881 18.239 1.00 42.51 AT ATOM 5904 0 HOH 305 35.383 27.547 41.161 1.00 46.62 ΔТ ATOM 5905 0 нон -1.325 306 41.441 28.735 1.00 43.36 ATOM 5906 0 нон 307 18.409 47.629 30.260 1.00 46.92 AT ATOM 5907 0 HOH 308 -0.365 41.851 31.323 1.00 43.06 ATOM 5908 0 нон 309 31.846 13.357 43.817 1.00 49.55 ATOM 5909 0 HOH 310 51.910 47.621 -1.442 1.00 43.27 ATOM 5910 0 HOH 311 29.562 44.918 17.110 1.00 52.42 AT ATOM 5911 нон 312 30.495 43.251 13.422 1.00 45.47 AT ATOM 5912 O HOH 313 11.474 10.744 42.423 1.00 51.55 ΔТ ATOM 5913 0 HOH 314 14.240 10.741 46.442 1.00 43.12 ΑT ATOM 5914 0 нон 315 52.861 58.416 6.793 1.00 44.59 AT ATOM 5915 O HOH 316 28.512 44.265 22.711 1.00 45.20 AT ATOM 5916 0 нон 317 72.643 46.339 -17.391 1.00 46.70 AΤ ATOM 5917 0 HOH 318 31.387 46,123 19.248 1.00 43.61 AT ATOM 5918 O HOH 319 78.102 45.702 -8.575 1.00 48.47 AT ATOM 5919 0 HOH 320 53.628 13.801

65.846

41.074

30.457

23.888

46.169

64.632

50.410

17.266

41.632

48.539

41.713

42.661

56.278

36.604

48.704

9.167

-7.173

27.174

20.027

19.783

15.804

-9.385

-3.435

4.657 48.965 1.00 55.69

1.00 49.46

1.00 44.55

1.00 50.50

1.00 47.21

1.00 49.37

1.00 51.43

1.00 48.35

1.00 48.93

AT

AT

AT

ΑT

AT

AT

AT

AT

AT



ATOM

ATOM

5982 0

5983 O

5984 O

HOH 384

HOH 385

HOH 386

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FIG. 1A-104

ATOM	5928	0	HOH	329	15.343	49.959	36.887	1.00		AT
ATOM	5929	0	HOH	330	77.778	42.870	3.924	1.00		AT
ATOM	5930	0	HOH	331	68.103	40.973	-5.266	1.00		TA
ATOM	5931	0	HOH	332	21.493	20.139	67.130	1.00		AΤ
ATOM	5932	0	HOH	333	81.269	24.355	14.982	1.00		AT
ATOM	5933	0	HOH	334	-5.903	30.538	26.686	1.00		PΑ
ATOM	5934	0	HOH	335	80.030	32.515	-0.810	1.00		AT
ATOM	5935	0	HOH	336	-7.205	27.318	42.127	1.00		AT
ATOM	5936	0	HOH	337	0.251	35.076	40.556	1.00		AT
ATOM	5937	0	HOH	338	67.263		-10.701	1.00		ΤA
ATOM	5938	0	HOH	339	78.930	41.885	0.871	1.00		AT
ATOM	5939	0	HOH	340	81.589	22.534	9.006	1.00		AT
ATOM	5940	0	HOH	341	-4.841	30.109	35.827	1.00		AT
ATOM	5941	0	HOH	342	24.216	28.828	53.120	1.00		AT
ATOM	5942	0	HOH	343	58.172		-15.457		37.88	AT
ATOM	5943	0	HOH	344	72.009		-12.680		44.56	TA
ATOM	5944	0	HOH	345	70.243		-16.741		37.48	TA
ATOM	5945	0	HOH	346	63.182		-22.683		47.83	AT
ATOM	5946	0	нон	347	59.201		-12.511		48.60	AT
ATOM	5947	0	HOH	348	73.024	32.150	-1.717		35.73	AT
ATOM	5948	0	HOH	349	36.241	17.553	55.406		43.52	AT
MOTA	5949	0	HOH	351	14.204	56.480	33.327		44.23	AT
ATOM	5950	0	HOH	352	81.607	27.771	16.204		46.37	AT
ATOM	5951	0	HOH	353	72.230	29.150	-2.863		44.64	AT
MOTA	5952	0	нон	354	63.965		-19.062		40.75	TA
MOTA	5953	0	нон	355	83.662	27.262	2.560		52.07	TA
ATOM	5954	0	нон	356	54.821	57.411	-7.143		47.42	AT
MOTA	5955	0	HOH	357	75.827	24.345	-2.592		38.53	AT
ATOM	5956	0	HOH	358	-3.100	29.989	33.712		35.26	AT
MOTA	5957	0	HOH	359	76.580	32.031	17.038		45.16	AT
MOTA	5958	0	HOH	360	61.004	63.374	-0.717		51.75	AT
ATOM	5959	0	нон	361	57.555		-17.566		37.15	TA
MOTA	5960	0	HOH	362	46.758	41.005	-9.571		49.08	AT
MOTA	5961	0	нон	363	65.046	41.921	10.931		43.73	AT
MOTA	5962	0	нон	364	60.495		-20.999		39.43	AT
MOTA	5963	0	нон	365	24.639	46.742	50.064		49.54	TA
MOTA	5964	0	нон	366	65.360		-12.244		42.08	AT
MOTA	5965	0	нон	367	81.253	38.379	6.191		44.60	TA TA
MOTA	5966	0	нон	368	20.278	58.789	32.999		51.96	
ATOM	5967	0	нон	369	35.754	25.608	43.846		41.69	AT AT
MOTA	5968	0	нон	370	58.812	30.456	20.182			AT
ATOM	5969	0	HOH	371	62.070	60.522			38.66 53.91	AT
ATOM	5970	0	нон	372	28.704	57.271	37.789		43.22	AT
ATOM ATOM	5971 5972	0	нон	373	16.768	31.252	63.214		45.45	AT
ATOM	5972		нон	374	17.431	24.978	67.168		57.67	AT
ATOM	5974	0	HOH	375	51.911	28.483	-4.087 15.354		48.16	AT
ATOM	5974	0	HOH	376 377	61.859	13.653	-7.635		40.72	AT
ATOM	5975	0	HOH	377	60.309	37.228	11.927		51.08	AT
ATOM	5976	0	HOH	378	76.341	49.000	49.436		50.11	AT
ATOM	5977	0	HOH	379	26.911 60.796	4.583	14.825		41.08	AT
ATOM	5979	0	HOH	381	64.912	34.210			54.13	AT
ATOM	5980	0	HOH	381	24.406	25.422	35.245		46.00	AT
ATOM	5981	0							48.67	AT
ATOM	2301	U	HOH	383	27.206	10.460	58.142	1.00	10.0/	A1

69.870 64.847 0.287 1.00 51.86

13.388 53.599 30.313 1.00 53.21

65.207 44.282 -23.032 1.00 44.87

ΑT

AT

AT



SUBCLASS

CLASS

ATOM

ATOM

ATOM

ATOM

ATOM

6037 O HOH 440

6038 O HOH 441

6039 O HOH 442

6040 O HOH 443

6041 O HOH 444

F. 6

C.

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FIG. 1A-105

ATOM 5985 0 HOH 387 23.812 43.965 31.871 1.00 51.01 AT ATOM 5986 0 HOH 388 27.925 56.723 25,402 1.00 50.91 ΑТ ATOM 5987 a HOH 389 22.429 53.122 37.372 1.00 40.24 AT ATOM 5988 0 HOH 390 20.340 37.818 64.894 1.00 43.91 ΔТ ATOM 5989 0 HOH 391 3.772 17.279 18.046 1.00 55.83 AT ATOM 5990 0 HOH 392 61.560 29.447 -8.011 1.00 48.85 AT ATOM 5991 0 HOH 393 40.737 49.676 12.185 1.00 48.28 AT ATOM 5992 HOH 394 47.566 44.388 26.446 1.00 47.81 AT ATOM 5993 0 HOH 395 62.091 37.019 27.629 1.00 53.63 ΔТ 0 ATOM 5994 HOH 396 45.170 49.972 14.734 1.00 52.56 ΑТ ATOM 5995 0 HOH 397 25.713 56.378 37.487 1.00 46.30 AT ATOM 5996 0 HOH 398 19.430 54.171 39.827 1.00 43.81 AT 5997 ATOM HOH 399 25.461 13.937 28.867 1.00 46.75 AT ATOM 5998 0 нон 400 65.078 42.400 27.343 1.00 58.24 AT ATOM 5999 0 HOH 401 15.750 35.665 16.140 1.00 49.43 AT ATOM 6000 HOH 402 30.823 49 012 9 778 1.00 49.25 ΑТ ATOM 6001 0 HOH 403 63.642 30.868 -6.737 1.00 63.10 AT ATOM 6002 0 HOH 404 -5.102 30.693 29.722 1.00 44.38 AT ATOM 6003 0 HOH 405 5.998 28.463 48.599 1.00 45.41 AT ATOM 6004 0 HOH 406 78.918 22.759 14.469 1.00 48.83 AT 14.615 ATOM 6005 HOH 407 67.800 -0.774 1.00 47.19 AT ATOM 6006 0 HOH 408 -8.454 30.970 25.750 1.00 52.46 AT ATOM: 6007 0 HOH 409 39.982 27.102 31.435 1.00 51.86 AT ATOM 6008 HOH 410 73.123 40.475 21.437 1.00 60.13 AT MOTA 6009 0 HOH 411 60.888 14.040 1.887 1.00 46.41 ΔΤ ATOM 6010 0 HOH 412 36.503 50.699 10.642 1.00 54.16 AT ATOM 6011 0 HOH 413 59.362 1.00 49.09 62.211 -6.530 AΤ ATOM 6012 0 HOH 414 28.103 13.240 52.474 1.00 47.88 ът ATOM 6013 HOH 415 32.010 21.506 60.871 1.00 51.04 AT ATOM 6014 0 HOH 416 35.534 13.760 51.867 1.00 48.76 AT ATOM 6015 0 HOH 417 40.198 51.587 23.313 1.00 47.59 ΔТ ATOM 0 HOH 418 32.582 27.322 18.391 1.00 59.17 AT ATOM 6017 0 HOH 419 70.979 43.580 -23.023 1.00 62.55 AT ATOM 6018 0 HOH 420 72.711 52.348 -21.252 1.00 55.53 ΔТ ATOM 6019 0 HOH 421 51.501 60.903 2.181 1.00 56.42 ΑT ATOM 6020 0 HOH 423 53.460 21.733 -0.240 1.00 63.43 ΔΤ ATOM 6021 0 HOH 424 55 865 19.944 -0.930 1.00 45.43 AT ATOM 6022 0 HOH 425 11.457 18.171 63.981 1.00 40.96 ΑT ATOM 6023 0 HOH 426 29.667 28.514 52.029 1.00 40.86 AT ATOM 6024 0 HOH 427 21.382 43.057 31.379 1.00 37.88 AT ATOM 6025 0 HOH 428 72.431 56.442 -14.816 1.00 38.78 ת מ ATOM 6026 0 HOH 429 13.645 35.387 57.232 1.00 45.75 ът ATOM 6027 0 нон 430 47.325 44.655 9.515 1.00 52.79 AT ATOM 6028 O HOH 1.00 53.71 431 12.413 9.161 45.090 AT ATOM 6029 0 HOH 432 69.847 -2.341 39.107 1.00 47.46 AT ATOM 6030 0 HOH 433 40.580 34.476 3.546 1.00 42.74 AT ATOM 6031 0 HOH 434 68.590 1.00 50.14 27.199 -5.061 ΔТ ATOM 6032 0 HOH 435 81.709 33.738 20.448 1.00 51.49 AT ATOM 6033 0 нон 436 21,276 6.862 53.221 1.00 43.81 AT ATOM 6034 0 HOH 437 63.959 28.541 24.084 1.00 48.89 AT ATOM 6035 0 HOH 438 44.540 42.464 26.796 1.00 45.92 AT ATOM 6036 0 HOH 439 26.430 1.00 41.22 12.510 54.374 AT

13 505

61.236

48.452

-6.734

68.689

42.803

27.483

32.235

17.777

11.054

49.080

-9.781

26.577

28.953

1.803

1.00 49.02

1.00 53.99

1.00 39.84

1.00 43.66

1.00 54.43

AT

AT

AT

AT

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FIG. 1A-106

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APPROVED O.G. FIG.

BY CLASS SUBCLASS
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ATOM	6042	0	HOH	445	64.733	8.182	7.092	1.00 51.11	AT
MOTA	6043	0	HOH	446	47.452	47.307	25.789	1.00 50.83	AT
ATOM	6044	0	HOH	447	-5.597	17.191	22.022	1.00 62.54	AT
ATOM	6045	0	HOH	448	34.703	54.274	40.793	1.00 43.46	AT
ATOM	6046	0	HOH	449	7.584	42.423	41.797	1.00 50.29	AT
ATOM	6047	0	HOH	450	68.745	9.611	12.516	1.00 44.55	AT
ATOM	6048	0	HOH	451	10.345	30.448	14.624	1.00 52.09	AT
ATOM	6049	0	нон	452	28.739	24.654	67.367	1.00 43.81	AT
ATOM	6050	0	нон	453	59.859	15.451	-0.538	1.00 50.23	AT
ATOM	6051	0	нон	454	9.715	22.615	40.260	1.00 55.68	AT
ATOM	6052	0	HOH	455	8.408	33.305	58.554	1.00 48.77	AT
ATOM	6053	0	HOH	456	82.808	20.346	7.688	1.00 64.19	AT
ATOM	6054	0	HOH	457	20.676	9.525	40.046	1.00 47.64	AT
ATOM	6055	0	HOH	458	12.300	21.911	45.521	1.00 55.95	AT
ATOM	6056	0	нон	459	12.849	37.059	54.956	1.00 47.15	AT
ATOM	6057	0	нон	460	18.947	37.315	56.296	1.00 55.87	AT
ATOM	6058	0	нон	461	42.279	43.046	32.215	1.00 55.34	AT
MOTA	6059	0	нон	462	58.113	60.078	-9.775	1.00 41.21	AT
MOTA	6060	0	нон	463	-4.882	24.186	43.569	1.00 49.34	AT
ATOM	6061	0	нон	464	2.275	30.894	44.638	1.00 49.59	AT
ATOM	6062	0	нон	465	11.908	42.581	46.538	1.00 54.17	AT
ATOM	6063	0	нон	466	25.196	30.973	68.678	1.00 54.36	AT
ATOM	6064	0	нон	467	55.729	18.620	-3.586	1.00 51.13	AT
MOTA	6065	0	нон	468	12.016	5.491	40.550	1.00 54.15	AT
ATOM	6066	0	нон	469	56.711	29.214	27.406	1.00 63.41	AT
ATOM	6067	0	HOH	470	56.150	18.575	3.127	1.00 57.43	AT
ATOM	6068	0	HOH	471	18.186	11.646	26.302	1.00 54.34	AT
ATOM ATOM	6069 6070	S1	DTT	1	74.181	38.187	-0.498	1.00 67.01	TTI
ATOM	6071	C1 C2	DTT	1	72.670	38.130	-1.524	1.00 67.92	TT1
ATOM	6071	02	DTT	1	72.656	36.968	-2.590	1.00 68.22	TT1
ATOM	6072	C3	DTT	1	71.393	37.023	-3.311	1.00 68.98	TT1
ATOM	6074	03	DTT	1	73.769	37.036	-3.768	1.00 67.93	TT1
ATOM	6075	C4	DTT	1	73.674	35.873	-4.701	1.00 67.85	TTI
ATOM	6076	S4	DTT	1	75.213 75.541	37.003 38.418	-3.287 -2.099	1.00 67.57	TT1
ATOM	6077	S1	DTT	2	54.935	53.026	7.820	1.00 67.52	TT1
ATOM	6078	Cl	DTT	2	53.759	51.637	7.760	1.00 53.56	TT2
ATOM	6079	C2	DTT	2	52.738	51.637	6.562	1.00 53.84	TT2
ATOM	6080	02	DTT	2	51.885	50.534	6.613	1.00 54.90 1.00 56.10	
ATOM	6081	Ċ3	DTT	2	51.681	52.940	6.568	1.00 54.93	TT2
ATOM	6082	03	DTT	2	50.780	52.918	5.376	1.00 55.43	TT2
ATOM	6083	C4	DTT	2	52.313	54.325	6.524	1.00 54.51	TT2
ATOM	6084	S4	DTT	2	53.485	54.549	7.971	1.00 54.31	TT2
ATOM	6085	Sı	DTT	3	9.841	19.197	19.765	1.00 46.94	TT3
ATOM	6086	Cl	DTT	3	8.080	19.681	19.855	1.00 44.23	TT3
ATOM	6087	C2	DTT	3	7.123	18.477	20.203	1.00 44.23	TT3
ATOM	6088	02	DTT	3	5.758	18.968	20.283	1.00 45.68	TT3
ATOM	6089	C3	DTT	3	7.023	17.285	19.113	1.00 46.42	TT3
ATOM	6090	03	DTT	3	6.110	16.195	19.567	1.00 49.11	TT3
ATOM	6091	C4	DTT	3	8.337	16.568	18.812	1.00 45.21	TT3
ATOM	6092	S4	DTT	3	9.629	17.785	18.211	1.00 44.44	TT3
ATOM	6093	Sı	DTT	4	19.785	34.825	23.721	1.00 49.21	TT4
ATOM	6094	Cl	DTT	4	19.784	36.095	25.038	1.00 49.59	TT4
ATOM	6095	C2	DTT	4	18.556	37.084	24.993	1.00 51.01	TT4
ATOM	6096	02	DTT	4	18.673	38.019	26.105	1.00 52.92	TT4
ATOM	6097	C3	DTT	4	18.440	38.051	23.699	1.00 50.89	TT4
ATOM	6098	03	DTT	4	17.234	38.926			TT4



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FIG. 1A-107

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ATOM	6099	C4	DTT	4	18.302	37.325	22.365	1.00 50.07	TT4
ATOM	6100	S4	DTT	4	19.750	36.164	22.087	1.00 49.50	
ATOM	6101	Sl	DTT	5	13.883	15.968	40.130	1.00 53.89	
ATOM	6102	Cl	DTT	5	12.694	17.323	39.827	1.00 54.86	
ATOM	6103	C2	DTT	5	11.608	17.502	40.955	1.00 55.83	
ATOM	6104	02	DTT	5	10.754	18.625	40.590	1.00 57.35	
ATOM	6105	C3	DTT	5	10.561	16.283	41.172	1.00 55.92	
ATOM	6106	03	DTT	5	9.597	16.559	42.278	1.00 56.47	
ATOM	6107	C4	DTT	5	11.194	14.953	41.564	1.00 55.56	
ATOM	6108	S4	DTT	5	12.443	14.418	40.274	1.00 55.31	
ATOM	6109	C1	GOL	6	25.840	30.485	23.369	1.00 60.12	
MOTA	6110	01	GOL	6	24.418	30.344	23.510	1.00 58.37	
ATOM	6111	C2	GOL	6	26.254	30.565	21.841	1.00 60.62	
ATOM	6112	02	GOL	6	26.921	31.825	21.610	1.00 61.53	
ATOM	6113	C3	GOL	6	25.019	30.470	20.890	1.00 60.48	
ATOM	6114	03	GOL	6	25.353	30.640	19.507	1.00 60.02	
ATOM	6115	C1	GOL	7	79.028	22.813	10.783	1.00 59.60	
ATOM	6116	01	GOL	7	78.201	22.510	11.912	1.00 61.71	
ATOM	6117	C2	GOL	7	79.615	24.278	10.893	1.00 59.54	
ATOM	6118	02	GOL	7	81.057	24.201	10.902	1.00 59.72	
ATOM	6119	C3	GOL	7	79.147	25.010	12.189	1.00 58.44	
ATOM	6120	03	GOL	7	79.958	26.145	12.514	1.00 56.91	
ATOM	6121	NA+1	NA1	1	63.339	31.566	-2.590	1.00 26.24	
MOTA	6122	NA+1	NA1	2	65.507	33.113	17.476	1.00 24.78	
ATOM	6123	NA+1	NA1	3	52.138	43.339	-0.467	1.00 31.32	
ATOM	6124	NA+1	NA1	4	11.564	27.003	46.250	1.00 28.57	
ATOM	6125	NA+1	NA1	5	22.858	38.903	45.868	1.00 35.79	
ATOM	6126	NA+1	NA1	6	12.049	37.399	33.606	1.00 30.07	
ATOM	6127	NA+1	NA1	7	52.399	30.404	9.576	1.00 28.65	
ATOM	6128	NA+1	NA1	8	61.322	58.273	-12.969	1.00 38.12	
ATOM		CL-1		9	74.315	48.004	-8.768	1.00 36.69	ONS
ATOM		CL-1		10	10.448	28.591	48.519	1.00 26.89	
ATOM		CL-1		11	49.897	29.847	8.163	1.00 28.28	ONS
ATOM		CL-1		12	68.370	32.685	17.763	1.00 30.08	ONS
ATOM		CL-1		13	21.352	41.348	46.322	1.00 33.00	ONS
ATOM		CL-1		14	21.514	34.817	28.080	1.00 20.85	ONS
ATOM		CL-1		15	70.235	40.020	0.588	1.00 21.12	ONS
ATOM		CL-1		16	55.303	48.583	9.136	1.00 22.36	ONS
ATOM		CL-1		17	61.816	29.359	-3.630	1.00 27.78	ONS
ATOM		CL-1		18	66.265	35.653	18.338	1.00 26.36	ONS
ATOM		CL-1		19	9.405	38.244	34.766	1.00 27.56	ONS
ATOM		CL-1		20	56.075	30.580	-5.205	1.00 30.76	ONS
ATOM		CL-1		21	51.184	42.277	-2.989	1.00 29.31	ONS
ATOM		CL-1		22	8.488	34.106	46.950	1.00 31.69	ONS
ATOM		CL-1		23	26.255	30.563	26.909	1.00 29.29	ONS
ATOM		CL-1		24	14.532	19.865	38.018	1.00 22.44	ONS
ATOM		CL-1		25	38.459	48.451	29.075	1.00 41.86	ONS
ATOM		CL-1		26	48.969	36.502	-2.659	1.00 32.79	ons
ATOM	6147	CL-1	CL1	27	19.241	17.587	34.034	1.00 29.08	ONS
END									



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FIG. 2

16.	SUBCLASS	
0.6. F	OLASS	
APPROVED	BY	DRAFTSHAW

		Atom							
		Type	Res.		<u>x</u>	<u>Y</u>	<u>z</u>	<u>occ</u> <u>B</u>	MOL
ATOM	1	С	GLY	1	3.531	2.676	31.918	1.00 23.54	ACPS
ATOM	2	0	GLY	1	2.877	3.712	32.042	1.00 24.07	ACPS
ATOM	3	N	GLY	1	3.058	2.705	29.459	1.00 25.97	ACPS
ATOM	4	CA	GLY	1	3.503	1.884	30.623	1.00 24.19	ACPS
ATOM	5	N	ILE	2	4.299	2.191	32.884	1.00 21.88	ACPS
ATOM	6	CA	ILE	2	4.396	2.857	34.180	1.00 20.22	ACPS
ATOM	7	CB	ILE	2	4.119	1.857	35.329	1.00 19.41	ACPS
ATOM	8	CG2	ILE	2	4.474	2.485	36.679	1.00 18.46	ACPS
ATOM	9	CG1	ILE	2	2.647	1.429	35.289	1.00 19.13	ACPS



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 2A-1

AFRIOVED 0.G. F1G.

8Y CLASS SUBCLASS
DRAFISHAN

ATOM	10	CD1	ILE	2	2.303	0.294	36.250	1.00 20.56	ACPS
ATOM	11	С	ILE	2	5.769	3.490	34.376	1.00 19.58	ACPS
ATOM	12	ō	ILE	2	6.798	2.827	34.223	1.00 19.75	ACPS
ATOM	13	N	TYR	3	5.779	4.780	34.704	1.00 18.83	ACPS
ATOM	14	CA	TYR	3	7.024	5.493	34.942	1.00 18.94	ACPS
ATOM	15	СВ	TYR	3	6.814	7.004	34.809	1.00 21.16	ACPS
ATOM	16	CG	TYR	3	8.059	7.808	35.103	1.00 23.30	ACPS
ATOM	17	CD1		3	9.164	7.761	34.246	1.00 24.81	ACPS
ATOM	18		TYR	3	10.326	8.486	34.525	1.00 25.94	ACPS
ATOM	19		TYR	3	8.145	8.601	36.246	1.00 24.18	ACPS
	20		TYR	3	9.297	9.329	36.534	1.00 25.63	ACPS
ATOM	21	CZ	TYR	3	10.384	9.267	35.672	1.00 26.92	ACPS
ATOM	22	OH	TYR	3	11.524	9.974	35.970	1.00 28.98	ACPS
ATOM		C	TYR	3	7.555	5.165	36.340	1.00 17.87	ACPS
ATOM	23	0	TYR	3	8.757	4.968	36.525	1.00 18.51	ACPS
ATOM	24		GLY	4	6.657	5.107	37.325	1.00 16.17	ACPS
ATOM	25	И	GLY	4	7.088	4.789	38.678	1.00 13.94	ACPS
MOTA	26	CA		4	5.937	4.643	39.657	1.00 13.19	ACPS
ATOM	27	C	GLY	4	4.819	5.094	39.387	1.00 13.25	ACPS
ATOM	28	0	GLY		6.217	4.001	40.794	1.00 12.43	ACPS
ATOM	29	N	ILE	5 5	5.209	3.822	41.841	1.00 11.10	ACPS
ATOM	30	CA	ILE		4.718	2.326	41.963	1.00 11.22	ACPS
MOTA	31	CB	ILE	5	4.718	1.793	40.572	1.00 12.21	ACPS
ATOM	32		ILE	5	5.785	1.441	42.619	1.00 11.21	ACPS
ATOM	33		ILE	5	5.785	-0.010	42.831	1.00 12.31	ACPS
ATOM	34		ILE	5		4.294	43.175	1.00 10.72	ACPS
ATOM	35	C	ILE	5	5.793	4.254	43.175	1.00 10.72	ACPS
ATOM	36	0	ILE	5	7.013	4.358	44.108	1.00 10.20	ACPS
ATOM	37	N	GLY	6	4.910		45.414	1.00 10.20	ACPS
ATOM	38	CA	GLY	6	5.347	5.102		1.00 10.17	ACPS
ATOM	39	С	GLY	6	4.348	4.762	46.503		ACPS
ATOM	40	0	GLY	6	3.139	4.776	46.261	1.00 9.96 1.00 9.09	ACPS
ATOM	41	N	LEU	7	4.859	4.459	47.697		ACPS
ATOM	42	CA	LEU	7	4.024	4.109	48.852	1.00 9.72 1.00 10.10	ACPS
ATOM	43	CB	LEU	7	4.058	2.588	49.078		ACPS
ATOM	44	CG	LEU	7	3.308	2.001	50.285	1.00 9.72 1.00 12.07	ACPS
ATOM	45		LEU	7	1.814	2.059	50.037		ACPS
ATOM	46		LEU	7	3.741	0.552	50.503	1.00 10.42	ACPS
ATOM	47	С	LEU	7	4.530	4.804	50.121	1.00 10.28	
ATOM	48	0	TEA	7	5.739	4.936	50.319	1.00 10.25	ACPS
ATOM	49	И	ASP	8	3.610	5.255	50.976	1.00 9.98	ACPS ACPS
ATOM	50	CA	ASP	8	4.024	5.871	52.230	1.00 9.91	
ATOM	51	CB	ASP	8	4.323	7.365	52.045	1.00 9.85	ACPS
ATOM	52	CG	ASP	8	5.223	7.887	53.128	1.00 11.38	ACPS
ATOM	5 3	OD1	ASP	8	4.723	8.465	5 4.110	1.00 12.14	ACPS
ATOM	54	OD2	ASP	8	6.439	7.672	53.003	1.00 13.58	ACPS
MOTA	55	C	ASP	8	2.997	5.715	53.338	1.00 9.65	ACPS
ATOM	56	0	ASP	8	1.792	5.822	53.101	1.00 10.65	ACPS
ATOM	57	N	ILE	9	3.479	5.447	54.551	1.00 9.53	ACPS
ATOM	58	CA	ILE	9	2.598	5.334	55.721	1.00 9.56	ACPS
ATOM	59	CB	ILE	9	2.634	3.913	56.338	1.00 9.26	ACPS
ATOM	60	CG2	ILE	9	1.780	3.890	57.602	1.00 10.57	ACPS
ATOM	61		ILE	9	2.101	2.881	55.338	1.00 9.47	ACPS
ATOM	62		ILE	9	2.215	1.426	55.815	1.00 10.23	ACPS
ATOM	63	c	ILE	9	3.142	6.361	56.717	1.00 9.80	ACPS
ATOM	64	ō	ILE	é	4.233	6.206	57.245	1.00 9.76	ACPS
ATOM	65	N	THR	10	2.375	7.423	56.941	1.00 9.46	ACPS
ATOM	66	CA	THR	10	2.768	8.527	57.819	1.00 10.38	ACPS
MI ON	00	~~	T-111		2.700	0.52,			



ATOM

123 CA SER 17

4.013

17.356

SUBCLASS

CLASS I

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SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 2A-2

2.428 57.089 1.00 10.26 ACPS 9.871 ATOM 67 СВ THR 10 10.050 55.997 1.00 11.15 ACPS 3.340 OG1 THR 10 ATOM 68 11.081 58.021 1.00 11.35 ACPS CG2 THR 10 2.527 ATOM 69 59.211 1.00 10.55 ACPS 8.453 THR 10 2.113 70 c ATOM ACPS THR 10 0.936 8.111 59.336 1.00 10.3B ATOM 71 0 8.773 60.246 1.00 10.75 ACPS 2.897 GLU 11 ATOM 72 N GLU 2.463 8.743 61.654 1.00 11.46 ACPS CA 11 ATOM 73 62.544 1.00 11.49 ACPS 3.708 8.583 CB GLU 11 ATOM 74 3.454 8.435 64.044 1.00 14.01 ACPS CG GLU 11 ATOM 75 7.005 64.449 1.00 16.01 ACPS 3.151 ATOM 76 CD GLU 11 3.674 6.084 63.791 1.00 17.38 ACPS OE1 GLU 11 77 ATOM 65.435 1.00 18.05 ACPS 2.417 6.807 ATOM 78 OE2 GLU 11 1.697 10.012 62.065 1.00 11.12 ACPS GLU 11 79 C ATOM ACPS 2.255 11.106 62.037 1.00 11.41 ATOM 80 0 GLU 11 1.00 11.46 ACPS 0.430 9.865 62.447 N LEU 12 ATOM 81 -0.383 11.026 62.848 1.00 12.27 ACPS 82 CA LEU 12 ATOM ACPS -1.785 10.582 63.305 1.00 12.68 CB LEU 12 ATOM 83 ACPS CG LEU 12 -2.751 10.062 62.234 1.00 13.69 ATOM 84 9.642 62.918 1.00 13.86 ACPS CD1 LEU 12 -4.049 ATOM 85 1.00 14.80 ACPS CD2 LEU 12 -3.039 11.140 61.183 ATOM 86 0.265 11.839 63.963 1.00 12.67 ACPS LEU 12 ATOM 87 C ACPS 0 LEU 12 0.270 13.066 63.915 1.00 12.56 MOTA 88 64.958 1.00 13.19 ACPS LYS 13 0.826 11.158 89 N ATOM ACPS 66.085 1.00 14.09 CA LYS 13 1.457 11.852 ATOM 90 1.00 15.99 67.165 ACPS CB LYS 13 1.878 10.851 91 ATOM 68.017 1.00 20.36 ACPS CG LYS 13 0.740 10.332 ATOM 92 69.197 1.00 23.47 ACPS 1.290 9.557 93 CD LYS 13 ATOM 70.261 1.00 25.28 ACPS 94 CE LYS 13 0.232 9.319 ATOM 71.473 1.00 26.94 ACPS 13 0.840 8.690 ATOM 95 N2 LYS ATOM C 13 2.665 12.693 65.685 1.00 13.56 ACPS 96 LYS 66.295 1.00 13.25 ACPS 2.924 13.738 ATOM 97 0 LYS 13 1.00 12.75 ATOM ARG 14 3.423 12.237 64.692 ACPS 98 N 13.009 64.233 1.00 13.17 ACPS ATOM 99 CA ARG 14 4.579 5.436 12.178 63.270 1.00 14.59 ACPS ATOM 100 CB ARG 14 12.936 62.661 1.00 17.45 ACPS CG ARG 14 6.598 ATOM 101 7.572 12.010 61.933 1.00 21.04 ACPS ATOM 102 CD ARG 14 12.770 61.254 1.00 23.74 ACPS 8.623 ATOM 103 NE ARG 14 8.689 12.966 59.939 1.00 25.19 ACPS 104 CZ ARG 14 ATOM 1.00 25.79 ACPS 7.768 12.450 59.134 ATOM 105 NH1 ARG 14 13.701 59.425 1.00 15.80 ACPS NH2 ARG 14 9.671 ATOM 106 14.296 63.547 1.00 13.10 ACPS ATOM 107 c ARG 14 4.100 1.00 13.21 ACPS 15.377 63.798 ATOM 108 0 ARG 14 4.636 1.00 11.73 62.678 ACPS ATOM 109 N ILE 15 3.099 14.181 1.00 12.13 ACPS 15.348 61.988 ATOM 110 CA ILE 15 2.559 ACPS ATOM 111 CB ILE 15 1.468 14.924 60.965 1.00 12.16 1.00 13.81 ACPS CG2 ILE 0.822 16.150 60.320 ATOM 112 15 ATTOM 113 CG1 ILE 15 2.095 14.050 59.875 1.00 13.13 ACPS ACPS ATOM 14.736 59.050 1.00 15.37 114 CD1 ILE 15 3.191 16.356 62.996 1.00 12.43 ACPS ATOM 115 С ILE 15 1.981 ACPS ATOM 116 TT.E 15 2.165 17.571 62.845 1.00 13.17 O 1.00 12.31 ACPS 117 N ALA 16 1.292 15.859 64.019 ATOM 65.038 1.00 13.48 ACPS ATOM 118 CA ALA 16 0.711 16.740 66.000 1.00 13.26 ACPS ATOM 119 CB ALA 16 -0.165 15.938 1.00 13.84 120 С ALA 16 1.812 17.456 65.811 ACPS ATOM 1.00 14.13 ACPS ATOM 121 0 ALA 16 1.679 18.631 66.159 N SER 2.902 16.752 66.089 1.00 13.89 ACPS ATOM 122 17 66.809 1.00 14.78 ACPS



SEP 0 9 2002

TECH CENTER 1600/2900

FIG. 2A-3

J.G. FIG.	CLASS SUBCLASS	
APPROVED	, ka	DRAFTSMAH

	124	CB	SER	17	5.041	16.291	67.199	1.00 14.52	ACPS
MOTA			SER	17	6.151	16.878	67.861	1.00 15.33	ACPS
ATOM	125	OG		17	4.686	18.440	65.971	1.00 15.57	ACPS
MOTA	126	С	SER		4.981	19.528	66.478	1.00 16.23	ACPS
ATOM	127	0	SER	17	4.933	18.163	64.694	1.00 15.86	ACPS
ATOM	128	N	MET	18			63.861	1.00 17.36	ACPS
ATOM	129	CA	MET	18	5.568	19.173			ACPS
ATOM	130	CB	MET	18	5.920	18.593	62.491	1.00 18.79	
MOTA	131	CG	MET	18	6.984	17.513	62.579	1.00 21.58	ACPS
ATOM	132	SD	MET	18	7.569	16.962	60.979	1.00 27.23	ACPS
ATOM	133	CE	MET	18	6.322	15.823	60.550	1.00 24.77	ACPS
ATOM	134	C	MET	18	4.679	20.408	63.724	1.00 18.05	ACPS
ATOM	135	ō	MET	18	5.171	21.537	63.720	1.00 17.78	ACPS
MOTA	136	N	ALA	19	3.371	20.200	63.637	1.00 17.79	ACPS
	137	CA	ALA	19	2.439	21.320	63.519	1.00 19.33	ACPS
MOTA		CB	ALA	19	1.047	20.810	63.161	1.00 18.47	ACPS
MOTA	138		ALA	19	2.391	22.119	64.827	1.00 20.49	ACPS
ATOM	139	С			2.124	23.324	64.820	1.00 21.87	ACPS
MOTA	140	0	ALA	19	2.655	21.446	65.944	1.00 21.04	ACPS
MOTA	141	N	GLY	20		22.112	67.234	1.00 22.79	ACPS
ATOM	142	CA	GLY	20	2.635		67.506	1.00 24.03	ACPS
ATOM	143	С	GLY	20	3.916	22.879			ACPS
MOTA	144	0	GLY	20	3.920	23.834	68.283	1.00 25.21	ACPS
MOTA	145	И	ARG	21	5.007	22.463	66.875	1.00 24.92	
MOTA	146	CA	ARG	21	6.286	23.135	67.062	1.00 26.49	ACPS
ATOM	147	CB	ARG	21	7.420	22.117	67.058	1.00 27.00	ACPS
ATOM	148	CG	ARG	21	7.376	21.144	68.216	1.00 28.19	ACPS
ATOM	149	CD	ARG	21	8.764	20.607	68.471	1.00 29.42	ACPS
MOTA	150	NE	ARG	21	9.667	21.695	68.835	1.00 30.12	ACPS
ATOM	151	CZ	ARG	21	10.993	21.603	68.834	1.00 29.99	ACPS
ATOM	152	NH1		21	11.727	22.650	69.183	1.00 30.82	ACPS
ATOM	153	NH2		21	11.584	20.469	68.481	1.00 30.49	ACPS
ATOM	154	C	ARG	21	6.559	24.208	66.006	1.00 27.49	ACPS
ATOM	155	ŏ	ARG	21	7.329	25.141	66.247	1.00 28.27	ACPS
ATOM	156	И	GLN	22	5.935	24.073	64.840	1.00 27.79	ACPS
	157	CA	GLN	22	6.103	25.039	63.757	1.00 28.18	ACPS
ATOM		CB	GLN	22	6.697	24.364	62.515	1.00 29.33	ACPS
ATOM	158	CG	GLN	22	8.186	24.075	62.625	1.00 30.67	ACPS
ATOM	159		GLN	22	8.839	23.775	61.284	1.00 31.99	ACPS
ATOM	160	CD			10.065	23.853	61.148	1.00 33.50	ACPS
ATOM	161		GLN	22			60.291	1.00 31.08	ACPS
MOTA	162		GLN	22	8.029	23.422	63.406	1.00 27.71	ACPS
ATOM	163	C	GLN	22	4.765	25.686		1.00 27.71	ACPS
ATOM	164	0	GLN	2 2	3.866	25.036	62.869		ACPS
ATOM	165	N	ALA	23	4.646	26.976	63.707	1.00 26.91	
ATOM	166	CA	ALA	23	3.420	27.721	63.453	1.00 25.59	ACPS
ATOM	167	CB	ALA	23	3.578	29.155	63.945	1.00 26.37	ACPS
ATOM	168	С	ALA	23	2.966	27.722	61.994	1.00 24.20	ACPS
ATOM	169	0	ALA	23	1.784	27.936	61.711	1.00 25.27	ACPS
ATOM	170	N	ARG	24	3.885	27.478	61.068	1.00 22.39	ACPS
ATOM	171	CA	ARG	24	3.519	27.481	59.655	1.00 20.64	ACPS
ATOM	172	CB	ARG	24	4.265	28.617	58.943	1.00 23.30	ACPS
ATOM	173	CG	ARG	24	4.063	29.987	59.612	1.00 26.19	ACPS
ATOM	174	CD	ARG	24	4.793	31.085	58.862	1.00 30.07	ACPS
	175	NE	ARG	24	4.710	32.403	59.493	1.00 32.13	ACPS
MOTA			ARG	24		32.879	60.363	1.00 32.86	ACPS
ATOM	176	cz			5.594		60.720	1.00 33.10	ACPS
ATOM	177		ARG	24	6.644	32.150		1.00 34.22	ACPS
MOTA	178		ARG	24	5.435	34.097	60.867	1.00 34.22	ACPS
MOTA	179	C	ARG	24	3.784	26.144	58.956		ACPS
ATOM	180	0	ARG	24	3.982	26.094	57.744	1.00 17.80	ACPS



SEP 0 9 2002

FIG. 2A-4

.16.	SUBCLASS	
0.6.1	Ci. A.35	
APPROVED	'n	DRAFTSHAN

				25	3.765	25.057	59.720	1.00 16.89	ACPS
MOTA	181	N	PHE	25	4.007	23.738	59.147	1.00 16.15	ACPS
ATOM	182	CA	PHE	25		22.664	60.246	1.00 16.22	ACPS
ATOM	183	CB	PHE	25	3.958			1.00 16.81	ACPS
ATOM	184	ÇG	PHE	25	4.308	21.282	59.757		
ATOM	185	CD1	PHE	25	3.357	20.271	59.754	1.00 17.39	ACPS
ATOM	186	CD2	PHE	25	5.577	21.008	59.255	1.00 16.97	ACPS
ATOM	187	CE1	PHE	25	3.662	19.001	59.253	1.00 18.39	ACPS
ATOM	188	CE2	PHE	25	5.892	19.737	5 8.752	1.00 18.24	ACPS
ATOM	189	CZ	PHE	25	4.930	18.737	58.753	1.00 17.96	ACPS
ATOM	190	С	PHE	25	3.038	23.370	58.0 15	1.00 15.11	ACPS
ATOM	191	0	PHE	25	3.464	22.840	56.988	1.00 14.64	ACPS
ATOM	192	N	ALA	26	1.748	23.646	58.196	1.00 15.46	ACPS
ATOM	193	CA	ALA	26	0.762	23.332	57.162	1.00 15.40	ACPS
ATOM	194	CB	ALA	26	-0.658	23.670	57.642	1.00 16.24	ACPS
ATOM	195	C	ALA	26	1.075	24.093	55.881	1.00 15.52	ACPS
ATOM	196	ō	ALA	26	0.941	23.551	54.787	1.00 14.18	ACPS
ATOM	197	N	GLU	27	1.512	25.345	56.011	1.00 14.73	ACPS
ATOM	198	CA	GLU	27	1.839	26.155	54.838	1.00 15.35	ACPS
ATOM	199	CB	GLU	27	2.041	27.619	55.236	1.00 16.37	ACPS
MOTA	200	CG	GLU	27	0.782	28.381	55.603	1.00 18.60	ACPS
ATOM	201	CD	GLU	27	0.176	27.956	56.927	1.00 19.31	ACPS
ATOM	202	OE1		27	0.899	27.430	57.796	1.00 19.16	ACPS
ATOM	203	OE2	GLU	27	-1.040	28.169	57.109	1.00 22.95	ACPS
ATOM	204	C	GLU	27	3.089	25.652	54.115	1.00 14.38	ACPS
ATOM	205	0	GLU	27	3.309	25.946	52.944	1.00 14.80	ACPS
ATOM	206	И	ARG	28	3.907	24.896	54.829	1.00 15.20	ACPS
ATOM	207	CA	ARG	28	5.119	24.330	54.268	1.00 16.00	ACPS
ATOM	208	CB	ARG	28	6.018	23.880	55.420	1.00 18.75	ACPS
ATOM	209	CG	ARG	28	7.335	23.289	55.015	1.00 22.72	ACPS
ATOM	210	CD	ARG	28	8.158	22.968	56.250	1.00 25.44	ACPS
ATOM	211	NE	ARG	28	9.461	22.432	55.890	1.00 28.04	ACPS
ATOM	212	cz	ARG	28	10.382	22.070	56.775	1.00 28.40	ACPS
ATOM	213		ARG	28	11.542	21.594	56.356	1.00 29.55	ACPS
ATOM	214		ARG	28	10.135	22.184	58.074	1.00 28.44	ACPS
	215	C	ARG	28	4.768	23.129	53.380	1.00 15.03	ACPS
ATOM	216	0	ARG	28	5.345	22.925	52.311	1.00 15.61	ACPS
ATOM		Ŋ	ILE	29	3.792	22.350	53.824	1.00 14.41	ACPS
ATOM	217 218	CA	ILE	29	3.396	21.137	53.112	1.00 14.00	ACPS
ATOM	219	CB	ILE	29	2.883	20.066	54.121	1.00 13.17	ACPS
ATOM ATOM	220		ILE	29	2.586	18.765	53.401	1.00 13.59	ACPS
	221		ILE	29	3.900	19.834	55.245	1.00 13.14	ACPS
ATOM	221		ILE	29	5.307	19.516	54 . 785	1.00 12.95	ACPS
ATOM ATOM	222	CDI	ILE	29	2.313	21.299	52.034	1.00 13.32	ACPS
	223	0	ILE	29	2.370	20.650	50.993	1.00 13.97	ACPS
MOTA			LEU	30	1.350	22.181	52.275	1.00 12.58	ACPS
MOTA	225	N CA	LEU	30	0.211	22.337	51.369	1.00 12.60	ACPS
MOTA	226					22.390	52.207	1.00 12.43	ACPS
ATOM	227	CB	LEU	30	-1.073	21.263	53.220	1.00 12.14	ACPS
ATOM	228	CG	LEU	30	-1.309			1.00 13.80	ACPS
MOTA	229		LEU	30	-2.536	21.595	54.057	1.00 12.77	ACPS
ATOM	230		LEU	30	-1.496	19.932	52.491	1.00 12.77	ACPS
MOTA	231	C	LEU	30	0.227	23.540	50.432	1.00 12.00	ACPS
MOTA	232	0	LEU	30	0.732	24.605	50.785		
MOTA	233	И	THR	31	-0.342	23.359	49.242	1.00 13.04	ACPS
MOTA	234	CA	THR	31	-0.456	24.450	48.265	1.00 13.14	ACPS
ATOM	235	CB	THR	31	-0.746	23.921	46.859	1.00 13.54	ACPS
ATOM	236		THR	31	-2.018	23.262	46.854	1.00 13.92	ACPS
ATOM	237	CG2	THR	31	0.313	22.937	46.429	1.00 14.69	ACPS



SEP 0 9 2002 JECH CENTER 1600/2800

FIG. 2A-5

APPROVED 12. F.1G. 6V 6V CLASS SUBGLASS DRAFTSHARE

ATOM	238	С	THR	31	-1.641	25.328	48.690	1.00 13.91	ACPS
ATOM	239	ō	THR	31	-2.374	24.980	49.617	1.00 13.14	ACPS
ATOM	240	N	ARG	32	-1.836	26.455	48.014	1.00 15.34	ACPS
ATOM	241	CA	ARG	32	-2.947	27.338	48.367	1.00 15.55	ACPS
ATOM	242	CB	ARG	32	-2.912	28.615	47.517	1.00 16.36	ACPS
ATOM	243	CG	ARG	32	-1.630	29.403	47.682	1.00 18.69	ACPS
ATOM	244	CD	ARG	32	-1.794	30.834	47.191	1.00 20.77	ACPS
ATOM	245	NE	ARG	32	-2.750	31.590	48.000	1.00 22.37	ACPS
ATOM	246	cz	ARG	32	-3.938	32.003	47.569	1.00 23.12	ACPS
ATOM	247	NHl	ARG	32	-4.326	31.738	46.330	1.00 23.58	ACPS
ATOM	248	NH2	ARG	32	-4.738	32.686	48.380	1.00 22.27	ACPS
ATOM	249	С	ARG	32	-4.296	26.646	48.205	1.00 15.92	ACPS
ATOM	250	0	ARG	32	-5.166	26.781	49.054	1.00 16.02	ACPS
ATOM	251	N	SER	33	-4.467	25.908	47.114	1.00 16.47	ACPS
ATOM	252	CA	SER	33	-5.717	25.183	46.863	1.00 16.46	ACPS
ATOM	253	CB	SER	33	-5.638	24.465	45.513	1.00 17.75	ACPS
ATOM	254	OG	SER	33	-6.833	23.77 2	45.224	1.00 24.08	ACPS
ATOM	255	С	SER	33	-5.981	24.154	47.967	1.00 16.53	ACPS
ATOM	256	0	SER	33	-7.115	23.963	48.404	1.00 16.86	ACPS
ATOM	257	N	GLU	34	-4.926	23.484	48.413	1.00 15.70	ACPS
ATOM	258	CA	GLU	34	-5.058	22.480	49.458	1.00 15.77	ACPS
ATOM	259	CB	GLU	34	-3.753	21.677	49.573	1.00 14.72	ACPS ACPS
ATOM	260	CG	GLU	34	-3.578	20.659	48.459	1.00 15.35	ACPS
ATOM	261	CD	GLU	34	-2.174	20.079	48.369	1.00 13.75 1.00 13.81	ACPS
ATOM	262		GLU	34	-2.023	19.029	47.719	1.00 13.81	ACPS
ATOM	263		GLU	34	-1.215	20.669	48.916	1.00 15.99	ACPS
ATOM	264	С	GLU	34	-5.397	23.134	50.789	1.00 15.99	ACPS
ATOM	265	0	GLU	34	-6.206	22.621	51.563 51.050	1.00 16.62	ACPS
ATOM	266	N	LEU	35	-4.781 -5.025	24.285 25.008	52.285	1.00 17.38	ACPS
ATOM	267	CA	LEU	35	-4.064	26.199	52.401	1.00 17.16	ACPS
ATOM	268	CB	LEU	35 35	-2.614	25.863	52.761	1.00 17.73	ACPS
ATOM	269	CG	LEU	35	-1.722	27.078	52.532	1.00 17.25	ACPS
ATOM	270		LEU	35	-2.547	25.405	54.212	1.00 17.05	ACPS
ATOM	271	CDZ	LEU	35	-6.462	25.499	52.380	1.00 18.36	ACPS
MOTA	272 273	0	LEU	35	-7.035	25.535	53.466	1.00 17.94	ACPS
MOTA MOTA	274	N	ASP	36	-7.049	25.866	51.248	1.00 19.36	ACPS
ATOM	275	CA	ASP	36	-8.419	26.361	51.264	1.00 21.62	ACPS
ATOM	276	CB	ASP	36	-8.866	26.738	49.845	1.00 22.68	ACPS
ATOM	277	CG	ASP	36	-9.949	27.806	49.836	1.00 24.19	ACPS
ATOM	278		ASP	36	-9.928	28.690	50.724	1.00 25.68	ACPS
ATOM	279		ASP	36	-10.807	27.773	48.927	1.00 24.47	ACPS
ATOM	280	c	ASP	36	-9.321	25.285	51.857	1.00 22.68	ACPS
ATOM	281	ō	ASP	36	-10.269	25.589	52.587	1.00 23.58	ACPS
ATOM	282	N	GLN	37	-9.003	24.024	51.572	1.00 22.62	ACPS
MOTA	283	CA	GLN	37	-9.784	22.899	52.087	1.00 23.62	ACPS
MOTA	284	CB	GLN	37	-9.514	21.653	51.236	1.00 24.76	ACPS
MOTA	285	CG	GLN	37	-9.899	21.812	49.769	1.00 26.90	ACPS
ATOM	286	CD	GLN	37	-9.264	20.761	48.867	1.00 29.15	ACPS
ATOM	287		GLN	37	-9.409	19.557	49.092	1.00 30.76	ACPS
ATOM	288		GLN	37	-8.556	21.215	47.836	1.00 30.60	ACPS
ATOM	289	С	GLN	37	-9.445	22.617	53.554	1.00 23.33	ACPS
ATOM	290	ō	GLN	37	-10.321	22.331	54.367	1.00 23.90	ACPS
ATOM	291	N	TYR	38	-8.161	22.711	53.876	1.00 22.41	ACPS
MOTA	292	CA	TYR	38	-7.644	22.474	55.222	1.00 22.14	ACPS
ATOM	293	СВ	TYR	38	-6.115	22.564	55.169	1.00 20.71	ACPS
ATOM	294	CG	TYR	38	-5.376	22.533	56.491	1.00 20.71	ACPS



SEP 0 9 2002 TECH CENTER 1600 (2000)

ACPS

FIG. 2A-6

38

-4.945 23.711 57.107 1.00 20.16

295 CD1 TYR ATOM

ATOM	295	CD1	TYR	38	-4.545	23.711			
ATOM	296	CE1	TYR	38	-4.180	23.677	58.276	1.00 21.07	ACPS
ATOM	297		TYR	38	-5.033	21.322	57.084	1.00 19.25	ACPS
ATOM	298		TYR	38	-4.275	21.276	58.246	1.00 20.56	ACPS
		CZ	TYR	38	-3.848	22.451	58.837	1.00 21.15	ACPS
MOTA	299	OH	TYR	38	-3.079	22.392	59.976	1.00 21.86	ACPS
ATOM	300				-8.191	23.441	56.270	1.00 22.57	ACPS
ATOM	301	С	TYR	38		23.031	57.357	1.00 21.64	ACPS
ATOM	302	0	TYR	38	-8.599		55.933	1.00 23.00	ACPS
MOTA	303	N	TYR	39	-8.201	24.727			ACPS
MOTA	304	CA	TYR	39	-8.669	25.750	56.854	1.00 23.93	ACPS
MOTA	305	CB	TYR	39	-8.540	27.139	56.212	1.00 24.42	
ATOM	306	CG	TYR	39	-7.117	27.588	55.948	1.00 25.39	ACPS
ATOM	307	CD1	TYR	39	-6.061	27.134	56.734	1.00 26.23	ACPS
ATOM	308	CE1	TYR	39	-4.763	27.590	56.525	1.00 27.45	ACPS
ATOM	309	CD2	TYR	39	-6.836	28.512	54.939	1.00 26.81	ACPS
ATOM	310	CE2	TYR	39	-5.540	28.979	54.726	1.00 26.80	ACPS
ATOM	311	CZ	TYR	39	-4.508	28.516	55.522	1.00 27.95	ACPS
ATOM	312	ОН	TYR	39	-3.224	28.999	55.337	1.00 28.86	ACPS
ATOM	313	c	TYR	39	-10.095	25.568	57.369	1.00 24.48	ACPS
ATOM	314	ō	TYR	39	-10.440	26.118	58.412	1.00 25.01	ACPS
ATOM	315	N	GLU	40	-10.916	24.802	56.656	1.00 24.88	ACPS
ATOM	316	CA	GLU	40	-12.307	24.591	57.067	1.00 26.05	ACPS
ATOM	317	CB	GLU	40	-13.180	24.249	55.854	1.00 27.82	ACPS
ATOM	318	CG	GLU	40	-13.036	25.174	54.661	1.00 30.61	ACPS
ATOM	319	CD	GLU	40	-14.017	24.833	53.551	1.00 31.77	ACPS
	320		GLU	40	-14.101	23.640	53.178	1.00 32.73	ACPS
ATOM	321		GLU	40	-14.697	25.756	53.050	1.00 33.34	ACPS
MOTA		C	GLU	40	-12.487	23.467	58.086	1.00 25.59	ACPS
ATOM	322		GLU	40	-13.581	23.280	58.618	1.00 26.05	ACPS
MOTA	323	0	LEU	41	-11.420	22.731	58.368	1.00 24.07	ACPS
MOTA	324	N CA	LEU	41	-11.509	21.584	59.266	1.00 22.24	ACPS
MOTA	325			41	-10.578	20.486	58.744	1.00 21.78	ACPS
ATOM	326	CB	LEU	41	-10.760	20.090	57.273	1.00 21.91	ACPS
ATOM	327	CG	LEU	41	-9.666	19.107	56.881	1.00 21.70	ACPS
MOTA	328		LEU		-12.126	19.474	57.058	1.00 22.12	ACPS
MOTA	329		LEU	41	-12.126	21.813	60.748	1.00 21.46	ACPS
ATOM	330	C	LEU	41		22.800	61.141	1.00 21.25	ACPS
MOTA	331	0	LEU	41	-10.614		61.567	1.00 21.01	ACPS
ATOM	332	И	SER	42	-11.693	20.873	63.009	1.00 20.67	ACPS
ATOM	333	CA	SER	42	-11.476			1.00 21.24	ACPS
ATOM	334	CB	SER	42	-12.319	19.865	63.716	1.00 20.80	ACPS
MOTA	335	OG	SER	42	-11.874	18.558	63.388	1.00 20.69	ACPS
ATOM	336	С	SER	42	-10.008	20.617	63.245	1.00 20.89	ACPS
ATOM	337	0	SER	42	-9.309	20.184	62.328		ACPS
ATOM	338	И	GLU	43	-9.540	20.834	64.469	1.00 19.62	ACPS
ATOM	339	CA	GLU	43	-8.146	20.568	64.815	1.00 19.23	
ATOM	340	CB	GLU	43	-7.932	20.830	66.312	1.00 20.39	ACPS
ATOM	341	CG	GLU	43	-6.524	20.541	66.843	1.00 22.14	ACPS
ATOM	342	CD	GLU	43	-6.452	20.617	68.366	1.00 23.47	ACPS
ATOM	343	OE1	GLU	43	-6.731	21.698	68.922	1.00 23.93	ACPS
ATOM	344	OE2	GLU	43	-6.118	19.594	69.004	1.00 24.66	ACPS
ATOM	345	С	GLU	43	-7.789	19.120	64.473	1.00 18.65	ACPS
ATOM	346	0	GLU	43	-6.755	18.849	63.864	1.00 18.62	ACPS
ATOM	347	N	LYS	44	-8.653	18.190	64.853	1.00 17.32	ACPS
ATOM	348	CA	LYS	44	-8.403	16.777	64.591	1.00 17.24	ACPS
ATOM	349	CB	LYS	44	-9.441	15.931	65.326	1.00 16.54	ACPS
ATOM	350	CG	LYS	44	-9.404	14.452	64.984	1.00 17.99	ACPS
ATOM	351	CD	LYS	44	-10.561	13.732	65.664	1.00 19.56	ACPS
ALON	221	-	213	**	10.551	2052			



SEP 0 9 2002

FIG. 2A-7

	SUBCLASS	
10.G. F	CLASS	
APPROVED	34	DRAFTSMAH

ATOM	352	CE	LYS	44	-10.691	12.285	65.205	1.00 19.17	ACPS
ATOM	353	NZ	LYS	44	-11.159	12.153	63.799	1.00 19.63	ACPS
MOTA	354	C	LYS	44	-8.413	16.431	63.099	1.00 16.56	ACPS
ATOM	355	0	LYS	44	-7.530	15.719	62.613	1.00 16.25	ACPS
ATOM	356	N	ARG	45	-9.412	16.923	62.375	1.00 16.89	ACPS
MOTA	357	CA	ARG	45	-9.507	16.641	60.947	1.00 17.08	ACPS
ATOM	358	CB	ARG	45	-10.849	17.131	60.400	1.00 19.32	ACPS
ATOM	359	CG	ARG	45	-12.053	16.345	60.910	1.00 21.73	ACPS
ATOM	360	CD	ARG	45	-12.092	14.927	60.336	1.00 25.16	ACPS
ATOM	361	NE	ARG	45	-13.304	14.213	60.741	1.00 28.95	ACPS
ATOM	362	CZ	ARG	45	-13.616	12.977	60.360	1.00 30.49	ACPS
ATOM	363	NHI	ARG	45	-14.743	12.419	60.783	1.00 31.89	ACPS
ATOM	364	NH2	ARG	45	-12.808	12.296	59.553	1.00 32.45	ACPS
ATOM	365	С	ARG	45	-8.353	17.284	60.189	1.00 16.29	ACPS
MOTA	366	0	ARG	45	-7.871	16.734	59.198	1.00 15.72	ACPS
ATOM	367	N	LYS	46	-7.917	18.455	60.644	1.00 15.52	ACPS
ATOM	368	CA	LYS	46	-6.796	19.128	60.009	1.00 15.32	ACPS
ATOM	369	CB	LYS	46	-6.449	20.429	60.746	1.00 15.53	ACPS
ATOM	370	CG	LYS	46	-7.232	21.666	60.320	1.00 18.65	ACPS
ATOM	371	CD	LYS	46	-6.678	22.887	61.051	1.00 20.77	ACPS
MOTA	372	CE	LYS	46	-7.201	24.203	60.485	1.00 22.56	ACPS
ATOM	373	NZ	LYS	46	-8.661	24.396	60.688	1.00 24.62	ACPS
ATOM	374	С	LYS	46	-5.584	18.207	60.036	1.00 14.61	ACPS
ATOM	375	0	LYS	46	-4.892	18.051	59.033	1.00 14.78	ACPS
ATOM	376	N	ASN	47	-5.320	17.602	61.190	1.00 14.97	ACPS
ATOM	377	CA	ASN	47	-4.174	16.711	61.329	1.00 14.85	ACPS
ATOM	378	CB	ASN	47	-4.064	16.233	62.783	1.00 16.85	ACPS
ATOM	379	CG	ASN	47	-2.877	15.317	63.008	1.00 19.82	ACPS
ATOM	380		ASN	47	-1.732	15.704	62.794	1.00 22.35	ACPS
ATOM	381		ASN	47	-3.149	14.093	63.439	1.00 21.62	ACPS
ATOM	382	C	ASN	47	-4.283	15.517	60.373	1.00 14.22	ACPS
ATOM	383	0	ASN	47	-3.312	15.159	59.702	1.00 13.37	ACPS
ATOM	384	И	GLU	48	-5.461	14.915	60.289	1.00 13.02	ACPS
MOTA	385	CA	GLU	48	-5.650	13.774	59.392	1.00 13.33	ACPS
ATOM	386	CB	GLU	48	-7.005	13.122	59.666	1.00 13.97	ACPS
ATOM ATOM	387 388	CG	GLU	48 48	-7.094 -8.518	12.540	61.075	1.00 17.87	ACPS
ATOM	389		GLU	48	-8.518	12.306	61.525	1.00 19.35	ACPS
ATOM	390		GLU	48	-9.449	11.814	62.657	1.00 22.50	ACPS
ATOM	391	C	GLU	48	-5.531	12.615 14.180	60.754 57.925	1.00 22.51 1.00 12.99	ACPS
ATOM	392	ō	GLU	48	-4.927	13.463	57.121	1.00 12.41	ACPS ACPS
ATOM	393	N	PHE	49	-6.098	15.331	57.573	1.00 12.16	ACPS
ATOM	394	CA	PHE	49	-6.015	15.818	56.204	1.00 12.16	ACPS
ATOM	395	СВ	PHE	49	-6.827	17.118	56.058	1.00 12.74	ACPS
ATOM	396	CG	PHE	49	-6.785	17.716	54.674	1.00 13.38	ACPS
ATOM	397		PHE	49	-7.742	17.710	53.724	1.00 13.30	ACPS
MOTA	398		PHE	49	-5.794	18.626	54.324	1.00 12.58	ACPS
ATOM	399		PHE	49	-7.710	17.950	52.449	1.00 14.47	ACPS
ATOM	400		PHE	49	-5.754	19.197	53.058	1.00 13.76	ACPS
ATOM	401	cz	PHE	49	-6.714	18.860	52.120	1.00 14.53	ACPS
ATOM	402	c	PHE	49	-4.549	16.076	55.846	1.00 11.65	ACPS
ATOM	403	ŏ	PHE	49	-4.059	15.616	54.809	1.00 11.65	ACPS
ATOM	404	N	LEU	50	-3.852	16.805		1.00 11.42	ACPS
ATOM	405	CA	LEU	50	-2.454	17.140	56.717	1.00 11.42	ACPS
ATOM	406	СВ	LEU	50	-2.454	18.075	56.489 57.597	1.00 11.33	ACPS
ATOM	407	CG	LEU	50				1.00 12.38	ACPS
ATOM	408		LEU	50	-0.473	18.512	57.597		
-11011	400	CDI	250	30	-0.131	19.277	56.323	1.00 14.40	ACPS



SEP 0 9 2002

FIG. 2A-8

G.	SUBCLASS	
0.6.FI	Ct 485 S	
APPROVED	λs	DRAFTSHAH

MOTA	409	CD2	LEU	50	- (
MOTA	410	C	LEU	50	- 1
ATOM	411	0	LEU	50	- (
ATOM	412	N	ALA	51	-1
ATOM	413	CA	ALA	51	- 2
ATOM	414	СВ	ALA	51	-:
	415	C	ALA	51	- 3
MOTA	416	0	ALA	51	- 0
MOTA			GLY	52	- 3
MOTA	417	N			-:
ATOM	418	CA	GLY	52 52	- :
ATOM	419	С	GLY		
MOTA	420	0	GLY	52	-:
ATOM	421	N	ARG	53	-2
ATOM	422	CA	ARG	53	-:
MOTA	423	CB	ARG	53	-:
ATOM	424	CG	ARG	53	-:
ATOM	425	CD	ARG	53	- 4
MOTA	426	NE	ARG	53	- 9
ATOM	427	CZ	ARG	53	- 6
ATOM	428	NHl	ARG	53	- (
ATOM	429	NH2	ARG	53	٠.
MOTA	430	C	ARG	53	
ATOM	431	0	ARG	53	- (
MOTA	432	N	PHE	54	- (
MOTA	433	CA	PHE	54	. :
MOTA	434	CB	PHE	54	:
ATOM	435	CG	PHE	54	
ATOM	436	CD1	PHE	54	
ATOM	437	CD2	PHE	54	
MOTA	438	CE1	PHE	54	
ATOM	439	CE2	PHE	54	
ATOM	440	CZ	PHE	54	3
ATOM	441	С	PHE	54	:
ATOM	442	0	PHE	54	
ATOM	443	N	ALA	55	
ATOM	444	CA	ALA	55	:
ATOM	445	CB	ALA	55	- (
ATOM	446	C	ALA	55	
ATOM	447	ō	ALA	55	:
ATOM	448	N	ALA	56	:
ATOM	449	CA	ALA	56	- (
ATOM	450	СВ	ALA	56	- (
ATOM	451	c	ALA	56	
ATOM	452	ō	ALA	56	
ATOM	453	N	LYS	57	:
ATOM	454	CA	LYS	57	
ATOM	455	CB	LYS	57	
ATOM	456	CG	LYS	57	:
	457	CD	LYS	57	:
ATOM					:
ATOM	458	CE	LYS	57	
ATOM	459	NZ	LYS	57	-
ATOM	460	C	LYS	57	
ATOM	461	0	LYS	57	!
MOTA	462	N	GLU	58	•
MOTA	463	CA	GLU	58	•
ATOM	464	CB	GLU	58	•
ATOM	465	CG	GLU	58	•

	-0.213	19.390	58.824	1.00	13.78	ACPS
	-1.573	15.900	56.413	1.00	10.56	ACPS
	-0.684	15.827	55.569	1.00	10.55	ACPS
	-1.806	14.936	57.301	1.00	10.65	ACPS
	-1.001	13.711	57,291	1.00	10.86	ACPS
	-1.330	12.847	58.510	1.00	10.65	ACPS
	-1.213	12.905	56.003	1.00	11.03	ACPS
	-0.274	12.296	55.481	1.00	10.16	ACPS
	-2.441	12.913	55.490	1.00	11.30	ACPS
	-2.742	12.186	54.267	1.00	11.27	ACPS
	-2.113	12.848	53.050	1.00	11.12	ACPS
		12.174	52.144	1.00	10.32	ACPS
	-1.635	14.177	53.026	1.00	10.73	ACPS
	-2.118		51.906	1.00	10.83	ACPS
	-1.521	14.896	51.943	1.00	11.05	ACPS
	-1.919	16.385	51.012	1.00	13.36	ACPS
	-3.089	16.756		1.00	14.65	ACPS
	-4.316	15.894	51.232		13.75	ACPS
	-5.419	16.229	50.322	1.00	14.79	ACPS
	-6.569	15.562	50.280	1.00	14.79	ACPS
	-6.761	14.525	51.087	1.00	15.39	ACPS
	-7.534	15.932	49.445	1.00	10.44	ACPS
	0.001	14.732	51.974	1.00	10.44	ACPS
	0.654	14.603	50.938 53.193	1.00	10.64	ACPS
	0.557	14.728	53.193	1.00	9.72	ACPS
	1.999	14.549	54.903	1.00	10.85	ACPS
	2.308	14.710	55.264	1.00	11.55	ACPS
	3 - 770	14.621 13.386	55.407	1.00	12.45	ACPS
	4.397		55.522	1.00	12.56	ACPS
	4.505	15.780	55.806	1.00	12.31	ACPS
	5.729 5.841	13.301 15.709	55.923	1.00	11.84	ACPS
		14.462	56.066	1.00	13.57	ACPS
	6.452 2.392	13.154	52.861	1.00	9.79	ACPS
	3.377	13.134	52.123	1.00	9.57	ACPS
	1.607	12.136	53.210	1.00	9.67	ACPS
	1.873	10.770	52.742	1.00	9.05	ACPS
	0.894	9.788	53.396	1.00	9.23	ACPS
	1.758	10.694	51.218	1.00	9.72	ACPS
	2.578	10.070	50.550	1.00	10.39	ACPS
	0.730	11.327	50.666	1.00	9.39	ACPS
	0.550	11.313	49.215	1.00	9.78	ACPS
	-0.759	12.014	48.846	1.00	10.10	ACPS
	1.728	11.969	48.487	1.00	9.83	ACPS
	2.158	11.479	47.451	1.00	10.05	ACPS
	2.242	13.077	49.026	1.00	9.72	ACPS
	3.361	13.758	48.388	1.00	10.49	ACPS
,	3.477	15.194	48.914	1.00	9.29	ACPS
,	2.243	16.015	48.546	1.00	9.85	ACPS
,	2.383	17.492	48.881	1.00	10.42	ACPS
	1.057	18.196	48.628	1.00	10.41	ACPS
		19.689	48.629	1.00	10.56	ACPS
,	1.214	12.986	48.549	1.00	10.05	ACPS
	4.668		47.632	1.00	11.38	ACPS
	5.501	12.992 12.322	49.687	1.00	10.76	ACPS
	4.863		49.846	1.00	10.03	ACPS
	6.073	11.513 11.064	51.304	1.00	10.79	ACPS
	6.270	12.221	52.234	1.00	12.67	ACPS
•	6.674	12.221	32.234	1.00		ACFO



SEP 0 9 2002 TECH CENTER 1600/2900

FIG. 2A-9



PPROVED O.G. FIG.

SY CLASS SUBCLASS
AFTSMAN

ATOM 467 CEI GLU 58 7.452 10.642 53.851 1.00 12.52 ACPS ATOM 468 OE2 GLU 58 8.343 12.641 53.905 1.00 14.76 ACPS ATOM 470 O GLU 58 5.969 10.307 48.903 1.00 10.01 4.76 ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.04 ACPS ATOM 473 CB ALA 59 4.596 8.622 47.844 1.00 10.19 ACPS ATOM 473 CB ALA 59 4.596 8.622 47.844 1.00 10.19 ACPS ATOM 473 CB ALA 59 4.596 8.622 47.844 1.00 10.19 ACPS ATOM 474 C ALA 59 4.866 9.100 46.415 1.00 11.21 ACPS ATOM 475 O ALA 59 4.866 9.100 46.415 1.00 11.21 ACPS ATOM 476 N PHE 60 4.377 10.289 46.071 1.00 11.07 ACPS ATOM 476 N PHE 60 4.614 10.824 44.735 1.00 11.41 ACPS ATOM 477 CA PHE 60 4.614 10.824 44.735 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.35 ACPS ATOM 478 CB PHE 60 3.492 12.439 42.057 1.00 11.31 ACPS ATOM 480 CDI PHE 60 3.481 12.810 43.191 1.00 11.93 ACPS ATOM 481 CD2 PHE 60 3.841 12.926 40.793 1.00 11.51 ACPS ATOM 482 CEI PHE 60 3.841 12.926 40.793 1.00 12.57 ACPS ATOM 483 CE2 PHE 60 3.841 12.926 40.793 1.00 12.57 ACPS ATOM 485 C PHE 60 4.921 13.794 40.671 1.00 12.35 ACPS ATOM 486 C PHE 60 4.921 13.794 40.671 1.00 12.35 ACPS ATOM 487 N SER 61 8.262 11.775 45.336 1.00 11.71 ACPS ATOM 487 N SER 61 8.262 11.775 45.336 1.00 11.71 ACPS ATOM 487 N SER 61 8.262 11.775 45.336 1.00 11.71 ACPS ATOM 497 C D SER 61 9.039 10.444 481 1.00 10.91 ACPS ATOM 498 CB SER 61 8.865 1.529 40.671 1.00 11.51 ACPS ATOM 497 CD LYS 62 8.584 6.402 48.888 1.00 11.07 ACPS ATOM 497 CD LYS 62 8.587 7.053 44.476 1.00 11.74 ACPS ATOM 497 CD LYS 62 8.587 7.053 44.476 1.00 11.75 ACPS ATOM 497 CD LYS 62 8.581 9.355 45.581 1.00 11.77 ACPS ATOM 497 CD LYS 62 8.581 9.355 45.581 1.00 11.77 ACPS ATOM 497 CD LYS 62 8.581 9.355 45.581 1.00 11.77 ACPS ATOM 501 C LYS 62 8.586 7.053 44.476 1.00 11.31 ACPS ATOM 501 C LYS 62 8.581 9.351 9.355 45.581 1.00 11.77 ACPS ATOM 501 C LYS 62 8.581 9.351 9.355 45.581 1.00 11.77 ACPS ATOM 501 C LYS 62 8.581 9.351 9.355 45.581 1.00 11.77 ACPS ATOM 501 C PHE 64 8.3	ATOM	466	CD	GLU	58	7.551	11.800	53.407	1.00 14.43	ACPS
ATOM 468 0E2 GLU 58 8.343 12.641 53.905 1.00 14.76 ACPS ATOM 470 0 GLU 58 6.960 10.307 48.903 1.00 10.10 ACPS ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.10 ACPS ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.10 ACPS ATOM 472 CA ALA 59 4.796 8.622 47.844 1.00 10.19 ACPS ATOM 473 CB ALA 59 4.866 9.100 46.415 1.00 11.21 ACPS ATOM 476 N PHE 60 4.877 10.289 46.071 1.00 10.97 ACPS ATOM 476 N PHE 60 4.571 10.289 46.071 1.00 10.97 ACPS ATOM 477 CA PHE 60 4.514 10.824 44.735 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.43 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.93 ACPS ATOM 478 CB PHE 60 3.948 12.182 40.571 1.00 10.97 ACPS ATOM 478 CB PHE 60 3.948 12.182 40.573 1.00 11.60 ACPS ATOM 480 CD1 PHE 60 3.492 12.439 42.057 1.00 11.51 ACPS ATOM 481 CD2 PHE 60 3.584 13.684 43.047 1.00 11.93 ACPS ATOM 482 CE1 PHE 60 3.841 12.926 40.793 1.00 12.35 ACPS ATOM 483 CE2 PHE 60 5.641 14.174 41.794 1.00 12.35 ACPS ATOM 485 C PHE 60 4.91 13.794 40.671 1.00 11.50 ACPS ATOM 485 C PHE 60 4.921 13.794 40.671 1.00 11.51 ACPS ATOM 486 C PHE 60 6.40 4.921 13.794 40.671 1.00 11.51 ACPS ATOM 487 N SER 61 6.828 11.529 45.483 1.00 11.07 ACPS ATOM 488 CA SER 61 8.815 12.510 46.561 1.00 11.55 ACPS ATOM 488 CA SER 61 8.826 11.775 45.336 1.00 11.17 ACPS ATOM 490 CS SER 61 9.039 10.703 43.390 1.00 11.17 ACPS ATOM 491 C SER 61 9.039 10.487 45.094 10.00 12.17 ACPS ATOM 492 C SER 61 9.039 10.487 45.094 10.00 12.17 ACPS ATOM 493 N LYS 62 8.513 9.365 44.594 1.00 11.56 ACPS ATOM 494 CA LYS 62 9.165 8.081 45.361 1.00 11.07 ACPS ATOM 495 C LYS 62 9.165 8.081 45.361 1.00 11.07 ACPS ATOM 496 C LYS 62 8.588 77.051 46.561 1.00 11.176 ACPS ATOM 497 C LYS 62 8.588 77.051 46.395 1.00 11.07 ACPS ATOM 498 C LYS 62 8.588 77.051 46.395 1.00 11.07 ACPS ATOM 496 C LYS 62 8.587 7.051 46.395 1.00 11.07 ACPS ATOM 500 C LYS 62 8.588 77.051 40.00 1.00 1.07 ACPS ATOM 501 C LYS 62 8.587 7.051 40.00 1.00 1.00 1.72 ACPS ATOM 501 C LYS 62 8.587 7.051 40.00 1.00 1.00 1.07 ACPS ATOM 501 C LYS 62 8.587 7						7.452	10.642	53.851	1.00 12.52	ACPS
ATOM 469 C GLU 58 5.969 10.307 48.903 1.00 10.19 ACPS ATOM 470 0 GLU 58 6.969 7.897 48.298 1.00 11.04 ACPS ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.50 ACPS ATOM 473 CPA ALA 59 4.596 8.622 47.844 1.00 10.050 ACPS ATOM 473 CPA ALA 59 4.596 8.622 47.844 1.00 10.91 ACPS ATOM 474 C ALA 59 4.866 9.100 46.415 1.00 11.21 ACPS ATOM 475 O ALA 59 4.866 9.100 45.641 1.00 11.07 ACPS ATOM 476 N PHE 60 4.377 10.289 46.071 1.00 10.97 ACPS ATOM 477 CA PHE 60 4.377 10.289 46.071 1.00 10.97 ACPS ATOM 478 CB PHE 60 3.918 12.881 44.735 1.00 11.13 ACPS ATOM 479 CG PHE 60 3.918 12.881 44.735 1.00 11.13 ACPS ATOM 479 CG PHE 60 3.492 12.439 42.057 1.00 11.35 ACPS ATOM 481 CD2 PHE 60 3.841 12.926 40.793 1.00 12.57 ACPS ATOM 481 CD2 PHE 60 3.841 12.926 40.793 1.00 12.57 ACPS ATOM 483 CE2 PHE 60 5.541 14.174 41.794 1.00 11.05 ACPS ATOM 483 CE2 PHE 60 5.641 14.174 41.794 1.00 11.05 ACPS ATOM 485 C PHE 60 6.109 11.014 44.481 1.00 10.91 ACPS ATOM 486 CP PHE 60 6.599 10.703 43.390 1.00 12.57 ATOM 487 N SER 61 6.828 11.529 45.483 1.00 11.17 ACPS ATOM 489 CB SER 61 8.815 12.510 46.561 1.00 11.07 ACPS ATOM 489 CB SER 61 8.815 12.510 46.561 1.00 11.07 ACPS ATOM 491 C SER 61 9.036 10.487 45.336 1.00 11.17 ACPS ATOM 493 N LYS 62 8.513 9.365 45.583 1.00 11.17 ACPS ATOM 495 CB LYS 62 9.155 8.891 1.00 3.395 1.00 12.17 ACPS ATOM 496 CD LYS 62 8.581 6.303 10.487 45.004 1.00 12.17 ACPS ATOM 497 CD LYS 62 8.581 6.303 10.08 1.00 11.07 ACPS ATOM 498 CB SER 61 8.262 11.775 45.336 1.00 11.07 ACPS ATOM 499 CB SER 61 8.262 11.775 45.336 1.00 11.07 ACPS ATOM 490 CG SER 61 9.039 10.703 40.671 1.00 11.56 ACPS ATOM 491 C SER 61 9.039 10.703 40.487 10.00 11.57 ACPS ATOM 495 CB LYS 62 8.584 6.402 48.888 1.00 8.91 ACPS ATOM 496 CB LYS 62 8.591 9.703 10.487 41.00 11.07 ACPS ATOM 497 CD LYS 62 8.591 9.703 10.487 41.00 11.07 ACPS ATOM 498 CB LYS 62 8.592 1.003 10.00 10.77 ACPS ATOM 500 C LYS 62 9.758 7.003 44.476 1.00 11.07 ACPS ATOM 501 C LYS 62 9.758 7.003 40.497 41.00 11.67 ACPS ATOM 501 C LYS 62 9.758 7.003 40.497 41.00 11.67 ACPS ATOM 501 C PHE 64 10.402 13.339						8.343	12.641	53.905	1.00 14.76	ACPS
ATOM 470 O GULU 58 6.960 9.897 48.298 1.00 11.04 ACPS ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.50 ACPS ATOM 472 CA ALA 59 4.596 8.622 47.844 1.00 10.19 ACPS ATOM 473 CB ALA 59 3.178 8.031 47.965 1.00 19.73 ACPS ATOM 474 C ALA 59 5.510 8.402 45.641 1.00 11.07 ACPS ATOM 476 N PHE 60 4.377 10.289 46.071 1.00 10.70 ACPS ATOM 476 N PHE 60 4.377 10.289 46.071 1.00 10.70 ACPS ATOM 477 CA PHE 60 4.614 10.824 44.735 1.00 11.41 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.536 1.00 11.35 ACPS ATOM 479 CG PHE 60 3.918 12.182 44.536 1.00 11.35 ACPS ATOM 480 CD PHE 60 3.492 12.439 42.057 1.00 11.93 ACPS ATOM 481 CD2 PHE 60 3.841 12.926 40.793 1.00 11.51 ACPS ATOM 482 CEI PHE 60 3.841 12.926 40.793 1.00 11.51 ACPS ATOM 483 CE2 PHE 60 5.641 1.174 41.794 1.00 12.57 ACPS ATOM 484 CZ PHE 60 4.921 13.794 40.671 1.00 11.51 ACPS ATOM 485 C PHE 60 6.599 10.703 43.390 1.00 11.17 ACPS ATOM 486 O PHE 60 6.599 10.703 43.390 1.00 11.17 ACPS ATOM 487 N SER 61 8.262 11.755 45.336 1.00 11.17 ACPS ATOM 490 CG SER 61 9.026 11.642 47.660 1.00 12.07 ACPS ATOM 491 C SER 61 8.262 11.755 45.336 1.00 11.17 ACPS ATOM 492 C SER 61 8.262 11.755 45.336 1.00 11.17 ACPS ATOM 493 N LYS 62 8.513 9.365 45.583 1.00 11.70 ACPS ATOM 494 C ALY 62 62 8.513 9.365 45.583 1.00 11.70 ACPS ATOM 495 C SER 61 8.262 11.775 45.336 1.00 11.17 ACPS ATOM 496 C SER 61 8.815 12.510 46.561 1.00 11.51 ACPS ATOM 497 C D LYS 62 8.587 61 8.394 10.487 1.00 12.07 ACPS ATOM 498 C SER 61 8.815 12.510 46.561 1.00 11.50 ACPS ATOM 499 C SER 61 9.039 10.487 45.094 1.00 12.17 ACPS ATOM 496 C C LYS 62 9.165 8.081 1.00 11.70 11.70 ACPS ATOM 497 C D LYS 62 8.587 61 8.394 1.00 11.07 ACPS ATOM 498 C SER 61 9.039 10.487 45.094 1.00 11.17 ACPS ATOM 499 C SER 61 9.039 10.487 45.094 1.00 11.10 ACPS ATOM 490 C SER 61 9.039 10.487 45.094 1.00 11.70 ACPS ATOM 500 C LYS 62 8.587 61 30.039 10.487 45.001 1.00 11.70 ACPS ATOM 501 C LYS 62 8.587 61 30.039 10.487 45.001 1.00 11.70 ACPS ATOM 501 C LYS 62 8.587 61 30.039 10.487 50.00 11.70 ACPS ATOM 501 C LYS 62 8.596 61 30.039 10.487 50.00 11.70 ACPS ATOM 501								48.903	1.00 10.19	ACPS
ATOM 471 N ALA 59 4.773 9.742 48.765 1.00 10.50 ACPS ATOM 473 CB ALA 59 4.596 8.622 47.844 1.00 10.19 ACPS ATOM 474 C ALA 59 3.178 8.031 47.965 1.00 9.73 ACPS ATOM 475 O ALA 59 5.510 8.402 45.641 1.00 11.21 ACPS ATOM 476 N PHE 60 4.377 10.289 46.071 1.00 10.97 ACPS ATOM 477 CA PHE 60 4.377 10.289 46.071 1.00 10.97 ACPS ATOM 478 CB PHE 60 3.918 12.182 44.735 1.00 11.41 ACPS ATOM 479 CG PHE 60 3.918 12.182 44.735 1.00 11.35 ACPS ATOM 479 CG PHE 60 3.918 12.810 43.191 1.00 11.35 ACPS ATOM 479 CG PHE 60 3.942 12.839 42.057 1.00 11.35 ACPS ATOM 481 CD2 PHE 60 5.284 13.684 43.047 1.00 11.51 ACPS ATOM 482 CE1 PHE 60 5.841 12.926 40.793 1.00 12.35 ACPS ATOM 483 CE2 PHE 60 5.641 14.174 41.794 1.00 12.35 ACPS ATOM 486 C PHE 60 4.921 13.794 40.671 1.00 11.05 ACPS ATOM 487 N SER 61 6.828 11.529 40.671 1.00 11.07 ACPS ATOM 488 CA SER 61 8.262 11.775 45.336 1.00 11.107 ACPS ATOM 488 CA SER 61 8.262 11.775 45.336 1.00 11.07 ACPS ATOM 490 OG SER 61 9.039 10.487 45.934 1.00 11.07 ACPS ATOM 491 C SER 61 9.039 10.487 45.934 1.00 11.07 ACPS ATOM 492 C SER 61 9.039 10.487 45.934 1.00 11.07 ACPS ATOM 493 N LYS 62 9.165 8.081 45.561 1.00 11.15 ACPS ATOM 496 CG LYS 62 9.165 8.081 45.561 1.00 11.15 ACPS ATOM 497 C SER 61 9.039 10.487 45.094 10.00 11.07 ACPS ATOM 498 C SER 61 8.865 12.510 46.561 1.00 11.07 ACPS ATOM 490 C SER 61 9.039 10.487 45.094 10.00 11.07 ACPS ATOM 491 C SER 61 9.039 10.487 45.094 10.00 11.07 ACPS ATOM 496 CG LYS 62 9.165 8.081 45.361 1.00 11.07 ACPS ATOM 497 CD LYS 62 8.513 9.365 45.583 1.00 11.07 ACPS ATOM 496 CG LYS 62 9.165 8.081 45.361 1.00 11.01 ACPS ATOM 497 CD LYS 62 8.513 9.365 45.583 1.00 11.07 ACPS ATOM 498 CE LYS 62 9.165 8.081 45.361 1.00 11.72 ACPS ATOM 496 CG LYS 62 9.165 8.081 45.361 1.00 11.72 ACPS ATOM 497 CD LYS 62 8.513 9.365 45.583 1.00 11.07 ACPS ATOM 498 CE LYS 62 8.513 9.365 40.451 1.00 11.72 ACPS ATOM 501 C LYS 62 8.584 6.00 40.93 10.487 50.00 10.07 ACPS ATOM 501 C PHE 64 9.039 10.487 7.00 10.00 10.07 ACPS ATOM 501 C PHE 64 9.039 10.487 7.00 10.00 10.07 ACPS ATOM 501 C PHE 64 9.039 10.487 7									1.00 11.04	ACPS
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ATOM 501 O LYS 62 9.758 7.062 43.264 1.00 12.36 ACPS ATOM 502 N ALA 63 7.642 7.815 43.472 1.00 12.11 ACPS ATOM 503 CA ALA 63 7.642 7.815 43.472 1.00 12.11 ACPS ATOM 504 CB ALA 63 7.266 7.408 42.119 1.00 12.83 ACPS ATOM 505 C ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATOM 506 O ALA 63 8.402 7.774 40.037 1.00 13.32 ACPS ATOM 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATOM 509 CB PHE 64 8.987 10.491 40.628 1.00 14.82 ACPS ATOM 509 CG PHE 64 8.856 11.878 41.290 1.00 14.92 ACPS ATOM 510 CG PHE 64 8.856 11.878 41.290 1.00 14.708 ACPS ATOM 510 CG PHE 64 8.715 13.350 39.253 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.57 ACPS ATOM 512 CD2 PHE 64 9.148 14.450 38.495 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.78 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.402 38.495 1.00 18.36 ACPS ATOM 517 O PHE 64 10.402 38.495 1.00 18.76 ACPS ATOM 518 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 519 C PHE 64 10.402 38.495 1.00 18.36 ACPS ATOM 510 C PHE 64 10.408 14.450 38.495 1.00 18.78 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 517 O PHE 64 10.402 38.907 41.655 1.00 14.55 ACPS ATOM 519 CA GLY 65 10.941 9.423 41.615 1.00 14.92 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 510 CG GLY 65 13.370 9.799 42.351 1.00 14.92 ACPS ATOM 510 CG GLY 65 13.370 9.799 42.351 1.00 14.92 ACPS	ATOM	499	NZ	LYS	62					
ATOM 502 N ALA 63 7.642 7.815 43.472 1.00 12.11 ACPS ATOM 503 CA ALA 63 7.266 7.408 42.119 1.00 12.83 ACPS ATOM 504 CB ALA 63 5.7551 7.567 41.914 1.00 11.67 ACPS ATOM 505 C ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATOM 506 O ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATOM 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATOM 508 CA PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATOM 510 CG PHE 64 8.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACPS ATOM 513 CE1 PHE 64 9.339 13.026 40.451 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 39.253 1.00 17.57 ACPS ATOM 515 CC PHE 64 10.402 13.809 40.805 1.00 18.89 ACPS ATOM 515 CC PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CC PHE 64 10.456 10.048 40.545 1.00 18.76 ACPS ATOM 515 CC PHE 64 10.456 10.048 40.545 1.00 18.36 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 18.86 ACPS ATOM 518 N GLY 65 10.941 9.423 11.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.348 1.00 15.63 ACPS ATOM 521 C GLY 65 13.370 9.729 42.348 1.00 15.63 ACPS ATOM 521 C GLY 65 13.370 9.729 42.348 1.00 15.63 ACPS	ATOM	500	C	LYS	62					
ATON 503 CA ALA 63 7.266 7.408 42.119 1.00 12.83 ACPS ATON 504 CB ALA 63 5.751 7.567 41.914 1.00 11.67 ACPS ATON 505 C ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATON 506 O ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATON 506 O ALA 63 8.402 7.774 40.037 1.00 13.32 ACPS ATON 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATON 509 CB PHE 64 8.987 10.491 40.628 1.00 14.82 ACPS ATON 509 CB PHE 64 8.987 10.491 40.628 1.00 14.82 ACPS ATON 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATON 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.08 ACPS ATON 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATON 513 CE1 PHE 64 9.148 14.450 38.495 1.00 17.57 ACPS ATON 513 CE1 PHE 64 10.802 13.809 40.885 1.00 18.78 ACPS ATON 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATON 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATON 516 C PHE 64 10.402 10.209 15.221 10.01 18.36 ACPS ATON 517 O PHE 64 10.402 10.209 39.547 1.00 16.68 ACPS ATON 518 N GLY 65 10.948 40.545 1.00 14.56 ACPS ATON 519 CA GLY 65 10.302 8.907 41.655 1.00 14.56 ACPS ATON 519 CA GLY 65 10.302 8.907 41.655 1.00 14.56 ACPS ATON 510 CG GLY 65 13.370 9.729 42.351 1.00 14.92 ATON 510 CG GLY 65 13.370 9.729 42.351 1.00 14.92 ATON 510 CG GLY 65 13.370 9.729 42.351 1.00 14.92	ATOM	501	0	LYS	62	9.758				
ATOM 504 CB ALA 63 5.751 7.567 41.914 1.00 11.67 ACPS ATOM 505 C ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATOM 506 O ALA 63 8.402 7.774 40.037 1.00 13.32 ACPS ATOM 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATOM 508 CA PHE 64 8.987 10.491 40.628 1.00 14.97 ACPS ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACPS ATOM 513 CE1 PHE 64 9.339 13.026 40.451 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.89 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.455 10.048 40.545 1.00 16.68 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS	ATOM	502	N	ALA	63					
ATON 505 C ALA 63 8.033 8.259 41.105 1.00 13.18 ACPS ATON 506 O ALA 63 8.402 7.774 40.037 1.00 13.18 ACPS ATON 506 O ALA 63 8.402 7.774 40.037 1.00 13.3.48 ACPS ATON 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATON 509 CB PHE 64 8.856 11.878 41.290 1.00 14.82 ACPS ATON 510 CG PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATON 511 CD1 PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATON 511 CD1 PHE 64 8.739 13.026 40.451 1.00 17.08 ACPS ATON 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATON 513 CE1 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATON 515 CZ PHE 64 10.838 14.904 40.137 1.00 18.78 ACPS ATON 515 CZ PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATON 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATON 516 C PHE 64 10.456 10.048 40.545 1.00 14.73 ACPS ATON 517 O PHE 64 10.456 10.048 40.545 1.00 14.73 ACPS ATON 517 O PHE 64 10.456 10.048 40.545 1.00 14.73 ACPS ATON 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATON 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATON 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATON 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATON 521 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS	ATOM	503	CA	ALA	63	7.266				
ATOM 506 O ALA 63 8.402 7.774 40.037 1.00 13.32 ACBS ATOM 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACBS ATOM 508 CA PHE 64 8.987 10.491 40.628 1.00 14.97 ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACBS ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACBS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACBS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACBS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACBS ATOM 513 CE1 PHE 64 10.402 13.809 40.885 1.00 18.78 ACBS ATOM 514 CE2 PHE 64 10.402 13.809 40.815 1.00 18.89 ACBS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACBS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACBS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACBS ATOM 518 N GUY 65 10.941 9.423 41.615 1.00 14.73 ACBS ATOM 519 CA GUY 65 12.302 8.907 41.652 1.00 14.56 ACBS ATOM 519 CA GUY 65 13.370 9.729 42.351 1.00 14.56 ACBS ATOM 521 O GUY 65 13.370 9.729 42.351 1.00 14.56 ACBS ATOM 521 O GUY 65 13.370 9.729 42.351 1.00 14.56 ACBS	ATOM	504	CB	ALA	63	5.751	7.567			
ATOM 507 N PHE 64 8.262 9.523 41.457 1.00 13.48 ACPS ATOM 508 CA PHE 64 8.987 10.491 40.628 1.00 14.82 ACPS ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATOM 510 CC PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACPS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.89 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.78 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.348 1.00 14.92 ACPS ATOM 521 O GLY 65 13.370 9.729 42.348 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63	ATOM	505	C	ALA	63	8.033	8.259			
ATOM 508 CA PHE 64 8.987 10.491 40.628 1.00 14.82 ACBS ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACBS ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACBS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACBS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.78 ACBS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACBS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACBS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACBS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACBS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACBS ATOM 518 N GUY 65 10.941 9.423 41.615 1.00 14.56 ACBS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACBS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACBS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.56 ACBS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACBS	ATOM	506	0	ALA	63	8.402	7.774			
ATOM 509 CB PHE 64 8.856 11.878 41.290 1.00 14.97 ACPS ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.78 ACPS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 17.57 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.86 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 18.78 ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63	ATOM	507	N	PHE	64	8.262	9.523	41.457		
ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.08 ACPS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.69 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 517 O PHE 64 10.406 40.545 1.00 14.67 ACPS ATOM 518 N GLY 65 10.048 40.545 1.00 14.67 ACPS ATOM 519 CA GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS	ATOM	508	CA	PHE	64	8.987	10.491	40.628		
ATOM 510 CG PHE 64 9.339 13.026 40.451 1.00 17.08 ACPS ATOM 511 CD1 PHE 64 8.715 13.350 39.253 1.00 17.75 ACPS ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 516 C PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 517 O PHE 64 10.405 10.048 40.545 1.00 14.77 ACPS ATOM 518 N GLY 65 10.948 40.545 1.00 14.67 ACPS ATOM 518 N GLY 65 10.948 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 10.948 41.615 1.00 14.73 ACPS ATOM 520 C GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 521 O GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS		509	CB	PHE	64	8.856	11.878	41.290	1.00 14.97	ACPS
ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 517 O PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.655 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS		510	CG	PHE	64	9.339	13.026	40.451		
ATOM 512 CD2 PHE 64 10.402 13.809 40.885 1.00 17.57 ACPS ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.56 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS	ATOM	511	CD1	PHE	64	8.715	13.350	39.253	1.00 17.78	
ATOM 513 CE1 PHE 64 9.148 14.450 38.495 1.00 18.78 ACPS ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS			CD2	PHE	64	10.402	13.809	40.885	1.00 17.57	ACPS
ATOM 514 CE2 PHE 64 10.838 14.904 40.137 1.00 18.89 ACPS ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.455 10.048 40.545 1.00 14.36 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS									1.00 18.78	ACPS
ATOM 515 CZ PHE 64 10.209 15.221 38.944 1.00 18.36 ACPS ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.56 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS									1.00 18.89	ACPS
ATOM 516 C PHE 64 10.456 10.048 40.545 1.00 14.87 ACPS ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.96 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										ACPS
ATOM 517 O PHE 64 11.136 10.290 39.547 1.00 16.68 ACPS ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.73 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										
ATOM 518 N GLY 65 10.941 9.423 41.615 1.00 14.73 ACPS ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										
ATOM 519 CA GLY 65 12.302 8.907 41.652 1.00 14.56 ACPS ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										
ATOM 520 C GLY 65 13.370 9.729 42.351 1.00 14.92 ACPS ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										
ATOM 521 O GLY 65 14.542 9.351 42.348 1.00 15.63 ACPS										
Alon Jal o dai da latera di latera d										
ATOM 522 N THR 66 12.979 10.826 42.980 1.00 16.03 ACPS										
	ATOM	522	N	THR	66	12.979	10.826	42.980	1.00 16.03	ACPS



SEP 0 9 2002 TECH CENTER 1600/2900

1.00 14.16

5.663 17.320 50.894 1.00 14.16 7.308 18.723 51.928 1.00 15.36

6.071 16.246 51.679 1.00 13.54

ACPS

ACPS

ACPS

TRADEMOS

577 CD1 PHE

578 CD2 PHE

579 CE1 PHE

ATOM MOTA

ATOM

74

74

74

APPROVED 0.15. F1G.

FIG. 2A-10

ATOM	523	CA	THR	66	13.945	11.700	43.643	1.00 16.17	ACPS
ATOM	524	CB	THR	66	13.908	13.103	43.038	1.00 17.57	ACPS
ATOM	525		THR	66	12.622	13.685	43.290	1.00 16.98	ACPS
ATOM	526	CG2	THR	66	14.150	13.056	41.531	1.00 18.71	ACPS
ATOM	527	c	THR	66	13.770	11.912	45.140	1.00 15.80	ACPS
ATOM	528	ŏ	THR	66	14.713	12.315	45.825	1.00 15.38	ACPS
ATOM	529	N	GLY	67	12.572	11.652	45.649	1.00 15.62	ACPS
ATOM	530	CA	GLY	67	12.319	11.918	47.052	1.00 15.38	ACPS
	531	c	GLY	67	12.088	13.421	47.173	1.00 15.61	ACPS
ATOM	532	ō	GLY	67	12.160	14.137	46.170	1.00 15.25	ACPS
ATOM	533	N	ILE	68	11.801	13.906	48.380	1.00 15.09	ACPS
	534	CA	ILE	68	11.580	15.332	48.598	1.00 16.65	ACPS
ATOM		CB	ILE	68	10.578	15.590	49.762	1.00 15.30	ACPS
ATOM	535		ILE	68	10.508	17.089	50.063	1.00 16.62	ACPS
ATOM	536		ILE	68	9.182	15.049	49.413	1.00 14.84	ACPS
MOTA	537	CD1	ILE	68	8.484	15.785	48.269	1.00 15.16	ACPS
ATOM	538 539	CDI	ILE	68	12.927	15.967	48.945	1.00 17.33	ACPS
ATOM	540	0	ILE	68	13.610	15.520	49.862	1.00 18.29	ACPS
ATOM	541	N	GLY	69	13.305	17.002	48.202	1.00 18.32	ACPS
ATOM ATOM	542	CA	GLY	69	14.574	17.663	48.436	1.00 20.27	ACPS
ATOM	543	C	GLY	69	14.877	18.700	47.371	1.00 20.85	ACPS
ATOM	544	0	GLY	69	13.990	19.447	46.949	1.00 20.98	ACPS
ATOM	545	N	ALA	70	16.128	18.734	46.920	1.00 22.02	ACPS
ATOM	546	CA	ALA	70	16.564	19.710	45.922	1.00 22.94	ACPS
ATOM	547	CB	ALA	70	18.064	19.575	45.690	1.00 24.19	ACPS
ATOM	548	C	ALA	70	15.834	19.655	44.582	1.00 23.39	ACPS
ATOM	549	ō	ALA	70	15.623	20.688	43.950	1.00 24.35	ACPS
ATOM	550	N	GLN	71	15.446	18.457	44.153	1.00 22.46	ACPS
ATOM	551	CA	GLN	71	14.765	18.289	42.871	1.00 21.53	ACPS
ATOM	552	CB	GLN	71	15.204	16.971	42.223	1.00 23.55	ACPS
ATOM	553	CG	GLN	71	16.683	16.924	41.843	1.00 26.32	ACPS
ATOM	554	CD	GLN	71	17.185	15.512	41.591	1.00 28.10	ACPS
ATOM	555		GLN	71	17.349	14.722	42.523	1.00 29.41	ACPS
ATOM	556	NE2	GLN	71	17.435	15.188	40.326	1.00 29.15	ACPS
ATOM	557	C	GLN	71	13.239	18.334	42.931	1.00 20.50	ACPS
ATOM	558	0	GLN	71	12.580	18.424	41.891	1.00 20.08	ACPS
ATOM	559	N	LEU	72	12.668	18.287	44.132	1.00 18.34	ACPS
ATOM	560	CA	LEU	72	11.210	18.292	44.261	1.00 16.54	ACPS
ATOM	561	CB	LEU	72	10.671	16.868	44.034	1.00 16.42	ACPS
ATOM	562	CG	LEU	72	9.146	16.682	44.035	1.00 15.69	ACPS
ATOM	563	CD1	LEU	72	8.539	17.358	42.815	1.00 16.49	ACPS
MOTA	564	CD2	LEU	72	8.811	15.186	44.032	1.00 16.39	ACPS
ATOM	565	С	LEU	72	10.752	18.786	45.632	1.00 15.95	ACPS
MOTA	566	0	LEU	72	11.177	18.260	46.654	1.00 16.86	ACPS
ATOM	567	N	SER	73	9.879	19.789	45.649	1.00 15.85	ACPS
ATOM	568	CA	SER	73	9.360	20.337	46.901	1.00 15.02	ACPS
ATOM	569	CB	SER	73	9.400	21.872	46.865	1.00 16.69	ACPS
MOTA	570	OG	SER	73	8.552	22.454	47.851	1.00 18.22	ACPS
MOTA	571	С	SER	73	7.920	19.896	47.122	1.00 13.98	ACPS
MOTA	572	0	SER	73	7.227	19.531	46.175	1.00 14.35	ACPS
ATOM	573	N	PHE	74	7.469	19.926	48.373	1.00 13.59	ACPS
ATOM	574	CA	PHE	74	6.083	19.584	48.674	1.00 12.78	ACPS
ATOM	575	СВ	PHE	74	5.802	19.731	50.177	1.00 12.70	ACPS
MOTA	576	CG	PHE	74	6.274	18.566	51.010	1.00 13.35	ACPS
3.000		an.	DITE	74		17 300	FA 004	1 00 14 16	ACDO



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FIG. 2A-11

TECH CENTER 1600/2900

ACPS

APPROVED O.C. FIG.
BY CLASS SUBCLASS
GRAFISMAN

17.653 52.720 CE2 PHE 74 7.727 1.00 14.73 580 ATOM 7.104 16.412 52.592 1.00 14.61 ATOM 581 СZ PHE 74 5.172 20.539 47.894 1.00 13.25 582 C PHE 74 ATOM 583 a PHE 74 4.070 20.179 47.500 1.00 13.15 ATOM 21.764 47.665 GLN 75 5.642 1.00 13.41 ATOM 584 N 585 CA GLN 75 4.848 22.749 46.929 1.00 13.12 ATOM 5.437 24.152 47.124 1.00 13.58 CB GLN 75 ATOM 586 75 5.338 24.667 48.545 1.00 14.20 587 CC GI.N ATOM 24.841 48.976 1.00 15.83 75 3.897 ATOM 588 CD GLN 3.077 25.355 48.217 1.00 17.10 589 OE1 GLN 75 ATOM 3.581 24.421 50.194 1.00 15.26 ATOM 590 NE2 GLN 75 4.701 22.473 1.00 13.39 75 45.430 ATOM 591 С GLN 3.865 23.097 44.769 1.00 14.75 ATOM 592 0 GLN 75 5.502 21.555 44.889 1.00 13.51 ATOM 593 N ASP 76 21.214 1.00 13.36 ATOM 594 CA ASP 76 5.423 43.464 6.760 20.670 42.950 1.00 14.98 595 CB ASP 76 ATOM 21.644 43.108 1.00 15.83 ATOM 596 CG ASP 76 7.907 7.682 22.872 43.049 1.00 17.92 597 OD1 ASP 76 ATOM ATOM 598 OD2 ASP 76 9.049 21.168 43,265 1.00 16.55 4.369 20.143 43.177 1.00 13.18 С ASP 76 ATOM 599 ATOM 600 0 ASP 76 4.138 19.781 42.016 1.00 13.17 3.743 19.637 44.234 1.00 12.89 601 N ILE 77 ATOM 602 CA TLE 77 2.765 18.561 44.116 1.00 12.84 ATOM CB ILE 77 3.248 17.339 44.932 1.00 11.96 ATOM 603 604 CG2 ILE 77 2.405 16.122 44.608 1.00 11.88 ATOM CG1 ILE 77 4.722 17.053 44.638 1.00 12.24 ATOM 605 606 CD1 ILE 77 5.413 16.211 45.724 1.00 12.11 ATOM 77 1.414 18.999 44.664 1.00 12.77 607 C TLE ATOM 608 0 ILE 77 1.330 19.552 45.766 1.00 13.68 ATOM 18.748 1.00 12.53 609 N GLU 78 0.349 43.910 ATOM CA GLU 78 -0.975 19.130 44.373 1.00 12.16 ATOM 610 611 CB GLU 78 -1.472 20.350 43.587 1.00 12.59 ATOM CG GLU 78 -2.722 20.983 44.167 1.00 13.40 ATOM 612 613 CD GLU 78 -2.987 22.339 43.559 1.00 14.46 ATOM 1.00 16.38 ATOM 614 OE1 GLU 78 -3.631 22.398 42.489 615 OE2 GLU 78 -2.524 23.340 44.147 1.00 15.90 ATOM 44.252 616 C GLU 78 -1.999 18.014 1.00 11.56 ATOM 1.00 12.82 ATOM 617 0 GLU 78 -2.145 17.402 43.198 618 N TLE 79 -2.704 17.748 45.344 1.00 11.82 ATOM ATOM 619 CA ILE 79 -3.750 16.734 45.329 1.00 12.32 ATOM 620 CB ILE 79 -3.893 16.000 46.698 1.00 12.41 ATOM 621 CG2 ILE 79 -5.201 15.191 46.723 1.00 12.50 ATOM 622 CG1 ILE 79 -2.737 15.010 46.913 1.00 11.83 ATOM 623 CD1 ILE 79 -1.372 15.660 47.132 1.00 12.95 45.048 ATOM 624 C ILE 79 -5.053 17.483 1.00 12.37 ATOM 625 0 ILE 79 -5.389 18.439 45.747 1.00 13.01 ATOM 626 N ARG 1.00 12.18 80 -5.753 17.059 44.003 ATOM 627 CA ARG 43.633 1.00 13.15 80 -7.037 17.649 ATOM 628 СВ ARG 80 -6.981 42.205 1.00 13.40 18.219 ATOM 629 CG ARG 80 -5.887 19.278 41.989 1.00 14.66 ATOM 630 CD ARG 80 -5.931 19.884 40.592 1.00 16.60 NE ATOM 631 ARG 80 -4.846 20.849 40.396 1.00 16.81 ATOM 632 CZ ARG 80 -4.588 21.471 39.248 1.00 18.53 ATOM 633 NH1 ARG 80 -3.581 39.175 1.00 18.94 22.331 ATOM 634 NH2 ARG 1.00 17.96 80 -5.331 21.240 38.173 1.00 13.09 ATOM 635 C ARG -8.061 16.516 43.701 80 ATOM o ARG 1.00 13.74 636 80 -7.697 15.352 43.882



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FIG. 2A-12

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ATPROVED O.C. FIG.
BY 91ASS SUBCLASS
DRAFTSKAN

637 N LYS ATOM ATOM 638 CA LYS 81 СВ LYS **R** 1 ATOM 639 CG LYS 81 ATOM 640 641 CD LYS 81 ATOM ATOM 642 CE LYS . 81 81 ATOM 643 NZ LYS ATOM 644 C LYS 81 81 ATOM 645 o LYS ATOM 646 N ASP 82 647 CA ASP 82 ATOM ATOM 648 CB ASP 82 649 CG ASP 82 ATOM ATOM 650 OD1 ASP 82 ATOM 651 OD2 ASP 82 652 C ASP 82 ATOM ATOM 653 0 ASP 82 ATOM 654 N GLN 83 655 CA GT.N 83 ATOM CB ATOM 656 GLN 83 ATOM 657 CG GLN 83 CD GLN ATOM 658 83 659 OE1 GLN 83 ATOM NE2 GLN 83 ATOM 660 661 c CT.N 83 ATOM 662 0 GI.N 83 ATOM 663 N D CN 84 ATOM 664 CA ASN 84 ATOM ATOM 665 CB ASN 84 ATOM 666 CG ASN 84 ATOM 667 OD1 ASN 84 ATOM 668 ND2 ASN 84 ATOM 669 C ASN 84 670 0 ASN 84 ATOM ATOM 671 Ν GLY 85 ATOM 672 CA GLY 85 ATOM 673 C GLY 85 ATOM 674 0 GLY 85 ATOM 675 N LYS 86 CA ATOM 676 LYS 86 ATOM 677 CB LYS 86 ATOM 678 CG LYS 86 ATOM 679 CD LYS 86 ATOM 680 CE LYS 86 ATOM 681 ΝZ LYS 86 ATOM 682 c LYS 86 ATOM 683 O LVS 86 ATOM 684 N PRO 87 ATOM 685 CD PRO 87 ATOM CD 686 PRO 87 ATOM 687 СВ PRO 87 ATOM 688 CG PRO 87 ATOM 689 C PRO 87 ATOM 690 0 PRO 87 ATOM 691 N TYR 88 ATOM 692 CA TYR 88 ATOM 693 TYR

43.577 1.00 13.78 81 -9.339 16.837 ACPS 43.610 -10.349 15.789 1.00 15.56 ACPS -10.943 15.648 45.017 1.00 17.86 ACPS -11.693 16.852 45.502 1.00 21.01 ACPS -12.183 16.669 46.939 1.00 23.45 ACPS 47.415 ACPS -12.982 17.886 1.00 25.03 -13.413 17.764 48.847 1.00 28.19 ACDS 16.080 42.612 ACPS -11.446 1.00 15.29 -11.752 17.249 42.329 1.00 15.96 ACPS -12.025 15.019 42.060 1.00 14.49 ACPS -13.102 15.191 41.102 1.00 13.96 ACPS 14.042 40.067 1.00 14.55 ACPS -13.140 -13.516 12.682 40.660 1.00 14.41 ACPS -14.130 12,609 41.738 1.00 13.41 ACPS 11.666 40.003 1.00 16.39 ACPS -13.199 -14.440 15.347 41.816 1.00 14.59 ACPS 15.366 43.048 1.00 13.66 ACPS -14.506 -15.506 15.464 41.03B 1.00 16.21 ACPS -16.836 15.671 41.596 1.00 18.34 ACPS -17.809 15.984 40.454 1.00 20.79 ACPS -17.344 17.201 39.649 1.00 25.58 ACPS -18.065 17.378 38.327 1.00 28.04 ACPS -17.669 18.207 37.505 1.00 30.79 ACPS -19.130 16.606 38.114 1.00 29.51 ACPS -17.351 14.530 42.465 1.00 18.31 ACPS -18.304 14.707 43.225 1.00 18.85 ACPS 42.363 1.00 18.00 ACPS -16.722 13.366 -17.126 12.220 43.178 1.00 18.03 ACPS 10.901 42.414 1.00 19.80 ACPS -16.984 -17.959 10.776 41.269 1.00 21.78 ACPS -19.160 10.993 41.432 1.00 24.79 ACPS -17.451 10.404 40.105 1.00 23.27 ACPS -16.282 12.111 44.439 1.00 16.61 ACPS -16.534 11.247 45.276 1.00 16.49 ACPS -15.278 12.972 44.568 1.00 15.58 ACPS -14.424 12.920 45.741 1.00 14.25 ACPS -13.153 12.107 45.539 1.00 14.48 ACPS 11.945 46.475 1.00 14.65 ACPS -12.368 -12.941 11.597 44.330 1.00 13.84 ACPS -11.741 10.810 44.042 1.00 12.93 ACPS -11.911 10.014 42.745 1.00 13.87 ACPS -10.672 9.204 42.353 1.00 15.94 ACPS -10.789 8.679 40.926 1.00 19.84 ACPS -9.548 7.906 40.485 1.00 20.40 ACPS -9.484 6.545 41.078 1.00 21.85 ACPS ACPS -10.534 11.730 43.883 1.00 13.03 43.078 1.00 12.98 ACPS -10.557 12,660 11.478 44.647 1.00 11.91 ACPS -9.461 -9.315 10.444 45.694 1.00 12.38 ACPS 1.00 11.87 ACPS -8.262 12.308 44.551 1.00 10.81 ACPS -7.556 12.043 45.874 ACPS -7.838 10.568 46.090 1.00 11.34 ACPS -7.386 11.913 43.377 1.00 11.68 1.00 11.62 ACPS -7.429 10.768 42.910 -6.615 42.895 1.00 11.62 ACPS 12.882 41.830 ACPS -5.639 12.674 1.00 11.77 88 1.00 13.03 ACPS -6.288 12.733 40.432



SEP 0 9 2002

FIG. 2A-13



ATOM	694	CG	TYR	88	-6.922	14.047	40.032	1.00 14.02	ACPS
ATOM	695		TYR	88	-6.188	15.023	39.364	1.00 14.07	ACPS
ATOM	696	CE1		88	-6.787	16.222	38.963	1.00 14.84	ACPS
ATOM	697	CD2		88	-8.271	14.298	40.294	1.00 14.32	ACPS
ATOM	698	CE2		88	-8.877	15.480	39.898	1.00 15.51	ACPS
ATOM	699	CZ	TYR	88	-8.131	16.442	39.232	1.00 15.27	ACPS
ATOM	700	OH	TYR	88	-8.728	17.622	38.835	1.00 17.40	ACPS
MOTA	701	С	TYR	88	-4.571	13.748	42.029	1.00 11.78	ACPS
MOTA	702	0	TYR	88	-4.801	14.752	42.698	1.00 11.93	ACPS
ATOM	703	N	ILE	89	-3.385	13.521	41.487	1.00 11.68	ACPS
ATOM	704	CA	ILE	89	-2.302	14.482	41.647	1.00 12.44	ACPS
ATOM	705	CB	ILE	89	-1.037	13.765	42.199	1.00 11.85	ACPS
ATOM	706		ILE	89	0.239	14.579	41.910	1.00 11.95	ACPS
ATOM	707		ILE	89	-1.185 -0.021	13.538 12.751	44.320	1.00 12.93	ACPS ACPS
ATOM	708		ILE	89	-1.921	15.214	40.371	1.00 12.53	ACPS
ATOM	709	C o	ILE	89 89	-2.000	14.662	39.271	1.00 12.52	ACPS
MOTA	710	N	ILE	90	-1.527	16.470	40.539	1.00 14.09	ACPS
ATOM	711 712	CA	ILE	90	-1.036	17.282	39.434	1.00 14.07	ACPS
ATOM ATOM	713	CB	ILE	90	-1.937	18.514	39.151	1.00 14.62	ACPS
ATOM	714	CG2		90	-1.254	19.433	38.127	1.00 15.25	ACPS
MOTA	715		ILE	90	-3.313	18.067	38.636	1.00 15.67	ACPS
MOTA	716	CD1		90	-3.289	17.301	37.330	1.00 16.06	ACPS
ATOM	717	C	ILE	90	0.357	17.780	39.855	1.00 14.28	ACPS
ATOM	718	ō	ILE	90	0.514	18.342	40.940	1.00 13.87	ACPS
ATOM	719	N	CYS	91	1.362	17.520	39.016	1.00 15.25	ACPS
ATOM	720	CA	CYS	91	2.737	17.974	39.242	1.00 15.44	ACPS
ATOM	721	CB	CYS	91	3.677	16.806	39.561	1.00 15.30	ACPS
ATOM	722	SG	CYS	91	5.404	17.317	39.841	1.00 14.62	ACPS
ATOM	723	C	CYS	91	3.139	18.606	37.916	1.00 16.53	ACPS
ATOM	724	0	CYS	91	3.585	17.926	36.990	1.00 17.19	ACPS
MOTA	725	N	THR	92	2.958	19.912	37.830	1.00 17.43	ACPS
ATOM	726	CA	THR	92	3.255	20.640	36.609	1.00 19.27	ACPS
ATOM	727	CB	THR	92	2.946	22.137	36.804	1.00 20.38	ACPS
ATOM	728	OG1	THR	92	1.550	22.286	37.117	1.00 22.97	ACPS
ATOM	729		THR	92	3.257	22.920	35.542	1.00 21.13	ACPS
MOTA	730	C	THR	92	4.685	20.436	36.102	1.00 19.66	ACPS
MOTA	731	0	THR	92	4.909	20.405	34.885	1.00 19.81	ACPS
MOTA	732	N	LYS	93	5.641	20.269	37.021	1.00 19.24	ACPS
ATOM	733	CA	LYS	93	7.040	20.049	36.633	1.00 20.40	ACPS
ATOM	734	CB	LYS	93	7.950	19.936	37.869	1.00 21.00	ACPS
ATOM	735	CG	LYS	93	8.283	21.253	38.540	1.00 23.04	ACPS
ATOM	736	CD	LYS	93	9.271	21.044	39.674	1.00 23.13	ACPS
ATOM	737	CE	LYS	93	9.590	22.347	40.394	1.00 25.70	ACPS
ATOM	738	NZ	LYS	93	10.683	22.160	41.393	1.00 27.21	ACPS
ATOM	739	C	LYS	93	7.194	18.774	35.816	1.00 19.95	ACPS
ATOM	740 741	O N	LYS	93	8.155	18.624	35.063	1.00 19.63	ACPS
ATOM	741	CA	LEU	94	6.251	17.851	35.978	1.00 20.99	ACPS
MOTA	742	CB	LEU	94	6.279	16.575	35.264		ACPS
ATOM	744	CG	LEU	94	5.643	15.485	36.129	1.00 23.41	ACPS
ATOM			LEU	94	5.579	14.064	35.563	1.00 24.26	ACPS
ATOM ATOM	745 746	CD1	LEU	94	6.980	13.493	35.405	1.00 26.39	ACPS
				94	4.761	13.194	36.507	1.00 25.01	ACPS
ATOM	747	C	LEU	94	5.530	16.674	33.936	1.00 23.14	ACPS
ATOM	748	0	LEU	94	6,110	16.499	32,862	1.00 22.82	ACPS
ATOM	749	N	SER	95	4.234	16.942	34.028	1.00 23.89	ACPS
ATOM	750	CA	SER	95	3.375	17.074	32.861	1.00 25.33	ACPS



SEP 0 9 2002

TECH CENTER 1600/2900

	ATOM	751	СВ	SER	95	3.268	15.736	32.112	1.00 26.52	ACPS
	ATOM	752	OG	SER	95	2.573	14.752	32.861	1.00 27.95	ACPS
	ATOM	753	c	SER	95	2.002	17.531	33.354	1.00 25.56	ACPS
	ATOM	754	ō	SER	95	1.760	17.599	34.561	1.00 24.02	ACPS
	ATOM	755	N	PRO	96	1.090	17.874	32.432	1.00 26.00	ACPS
	ATOM	756	CD	PRO	96	1.289	18.101	30.986	1.00 26.52	ACPS
	ATOM	757	CA	PRO	96	-0.240	18.324	32.853	1.00 25.75	ACPS
	ATOM	758	CB	PRO	96	-0.709	19.147	31.657	1.00 26.31	ACPS
	ATOM	759	CG	PRO	96	-0.119	18.392	30.506	1.00 26.75	ACPS
	MOTA	760	c	PRO	96	-1.201	17.179	33.176	1.00 25.06	ACPS
	ATOM	761	ō	PRO	96	-2.304	17.414	33.664	1.00 25.74	ACPS
	ATOM	762	N	ALA	97	-0.773	15.950	32.907	1.00 24.25	ACPS
1	ATOM	763	CA	ALA	97	-1.599	14.769	33.142	1.00 23.20	ACPS
1		764	CB	ALA	97	-0.967	13.555	32.479	1.00 24.01	ACPS
1	ATOM	765	C	ALA	97	-1.872	14.463	34.611	1.00 22.43	ACPS
	ATOM	766	0	ALA	97	-1.072	14.786	35.490	1.00 22.83	ACPS
	ATOM	767	N	ALA	98	-3.020	13.841	34.865	1.00 21.00	ACPS
	ATOM	768	CA	ALA	98	-3.411	13.462	36.215	1.00 19.60	ACPS
	ATOM	769	CB	ALA	98	-4.914	13.140	36.259	1.00 19.71	ACPS
	ATOM	770	C	ALA	98	-2.597	12.232	36.601	1.00 18.50	ACPS
	ATOM ATOM	771	0	ALA	98	-2.426	11.313	35.796	1.00 19.87	ACPS
	MOTA	772	N	VAL	99	-2.084	12.231	37.826	1.00 15.98	ACPS
	ATOM	773	CA	VAL	99	-1.299	11.120	38.346	1.00 14.14	ACPS
	ATOM	774	CB	VAL	99	-0.042	11.661	39.041	1.00 15.01	ACPS
	ATOM	775		VAL	99	0.630	10.575	39.854	1.00 15.26	ACPS
	ATOM	776		VAL	99	0.909	12.221	37.990	1.00 14.69	ACPS
	ATOM	777	C	VAL	99	-2.192	10.357	39.336	1.00 13.62	ACPS
	ATOM	778	0	VAL	99	-2.935	10.971	40.098	1.00 14.19	ACPS
	ATOM	779	N	HIS	100	-2.132	9.029	39.306	1.00 12.36	ACPS
	ATOM	780	CA	HIS	100	-2.949	8.192	40.178	1.00 12.74	ACPS
	ATOM	781	CB	HIS	100	-2.894	6.741	39.708	1.00 13.48	ACPS
	ATOM	782	CG	HIS	100	-3.505	6.514	38.362	1.00 14.92	ACPS
	ATOM	783	CD2		100	-2.938	6.353	37.143	1.00 15.96	ACPS
	ATOM	784	ND1		100	-4.868	6.432	38.165	1.00 15.90	ACPS
	ATOM	785	CE1		100	-5.113	6.232	36.883	1.00 17.29	ACPS
	ATOM	786	NE2		100	-3.960	6.181	36.241	1.00 15.85	ACPS
	ATOM	787	C	HIS	100	-2.513	8.233	41.630	1.00 12.24	ACPS
	ATOM	788	ō	HIS	100	-1.328	8.140	41.927	1.00 12.33	ACPS
	ATOM	789	N	VAL	101	-3.487	8.363	42.525	1.00 11.72	ACPS
	ATOM	790	CA	VAL	101	-3.217	8.365	43.958	1.00 11.15	ACPS
	ATOM	791	CB	VAL	101	-2.899	9.811	44.477	1.00 11.69	ACPS
	ATOM	792	CG1		101	-4.142	10.694	44.373	1.00 12.75	ACPS
	ATOM	793	CG2		101	-2.391	9.758	45.924	1.00 12.34	ACPS
	ATOM	794	C	VAL	101	-4.430	7.815	44.725	1.00 10.53	ACPS
	ATOM	795	ō	VAL	101	-5.565	7.914	44.253	1.00 10.71	ACPS
	ATOM	796	N	SER	102	-4.174	7.176	45.871	1.00 9.38	ACPS
	ATOM	797	CA	SER	102	-5.243	6.698	46.748	1.00 9.83	ACPS
	ATOM	798	CB	SER				46.517	1.00 10.13	ACPS
	ATOM	799	OG	SER	102 102	-5.574	5.218	47.295	1.00 9.75	ACPS
		800	C			-6.713	4.863		1.00 9.45	ACPS
	ATOM			SER	102	-4.782	6.906	48.192	1.00 10.30	ACPS
	ATOM	801	0	SER	102	-3.608	6.730	48.493		
	ATCM	802	N	ILE	103	-5.712	7.277	49.071	1.00 9.23	ACPS
	ATOM	803	CA	ILE	103	-5.417	7.563	50.474	1.00 9.67	ACPS
	ATOM	804	CB	ILE	103	-5.683	9.063	50.774	1.00 9.72	ACPS
	ATOM	805	CG2		103	-5.495	9.382	52.283	1.00 8.94	ACPS
	ATOM	806	CG1	ILE	103	-4.778	9.912	49.885	1.00 10.44	ACPS

-5.088 11.421 49.938 1.00 11.38

ACPS

ATCM 807 CD1 ILE 103

FIG. 2A-14



SEP 0 9 2002

FIG. 2A-15

TECH CENTER 1600/2900

APPROVED OF FIG.

ATOM	808	С	ILE	103	-6.299	6.728	51.388	1.00 9.74	ACPS
ATOM	809	0	ILE	103	-7.447	6.432	51.041	1.00 9.47	ACPS
ATOM	810	N	THR	104	-5.751	6.334	52.541	1.00 9.43	ACPS
ATOM	811	CA	THR	104	-6.507	5.567	53.537	1.00 9.07	ACPS
ATOM	812	CB	THR	104	-6.323	4.034	53.329	1.00 9.49	ACPS
ATOM	813	OG1	THR	104	-7.164	3.312	54.246	1.00 10.14	ACPS
ATOM	814	CG2	THR	104	-4.878	3.617	53.528	1.00 8.69	ACPS
ATOM	815	С	THR	104	-6.067	5.976	54.949	1.00 9.89	ACPS
ATOM	816	0	THR	104	-4.896	6.283	55.174	1.00 9.73	ACPS
ATOM	817	N	HIS	105	-7.006	5.978	55.891	1.00 10.13	ACPS
ATOM	818	CA	HIS	105	-6.734	6.384	57.266	1.00 10.93	ACPS
ATOM	819	CB	HIS	105	-7.632	7.572	57.622	1.00 11.25	ACPS
ATOM	820	CG	HIS	105	-7.371	8.805	56.817	1.00 11.60	ACPS
ATOM	821	CD2	HIS	105	-7.921	9.254	55.663	1.00 13.08	ACPS
MOTA	822	ND1	HIS	105	-6.442	9.749	57.192	1.00 11.93	ACPS
ATOM	823	CE1	HIS	105	-6.427	10.729	56.305	1.00 11.86	ACPS
ATOM	824	NE2	HIS	105	-7.315	10.451	55.366	1.00 12.18	ACPS
ATOM	825	C	HIS	105	-6.986	5.299	58.314	1.00 11.03	ACPS
ATOM	826	0	HIS	105	-7.888	4.471	58.165	1.00 12.54	ACPS
ATOM	827	N	THR	106	-6.165	5.309	59.367	1.00 11.51	ACPS
MOTA	828	CA	THR	106	-6.349	4.411	60.509	1.00 11.59	ACPS
ATOM	829	CB	THR	106	-5.289	3.270	60.620	1.00 11.24	ACPS
ATOM	830	OG1		106	-4.065	3.780	61.169	1.00 11.20	ACPS
ATOM	831	CG2		106	-5.01 7	2.634	59.261	1.00 12.65	ACPS
ATOM	832	С	THR	106	-6.225	5.273	61.771	1.00 12.23	ACPS
MOTA	833	0	THR	106	-6.002	6.482	61.692	1.00 12.54	ACPS
MOTA	834	N	LYS	107	-6.364	4.634	62.929	1.00 12.39	ACPS
ATOM	835	CA	LYS	107	-6. 269	5.295	64.229	1.00 12.12	ACPS ACPS
ATOM	836	CB	LYS	107	-6.473	4.242	65.326	1.00 12.29	ACPS
ATOM	837	CG	LYS	107	-5.379	3.146	65.280		ACPS
MOTA	838	CD	LYS	107	-5.653	1.939	66.203 65.876	1.00 14.42	ACPS
ATOM	839	CE	LYS	107	-4.660	0.799	66.648	1.00 18.55	ACPS
ATOM	840	NZ	LYS	107	-4.895	-0.473	64.490	1.00 12.43	ACPS
MOTA	841	С	LYS	107	-4.936 -4.874	5.998 6.970	65.263	1.00 14.30	ACPS
ATOM	842	0	LYS	107			63.857	1.00 11.38	ACPS
ATOM	843	N	GLU	108	-3.871	5.516 6.061	64.099	1.00 11.08	ACPS
ATOM	844	CA	GLU	108	-2.540 -1.692	4.997	64.823	1.00 10.76	ACPS
ATOM	845	CB	GLU	108	-1.320	3.790	63.936	1.00 11.72	ACPS
ATOM	846		GLU	108	-0.835	2.550	64.706	1.00 11.82	ACPS
MOTA	847	CD	GLU		-0.035	2.673	65.664	1.00 12.16	ACPS
MOTA	848	OE2		108 108	-1.224	1.420	64.329	1.00 11.39	ACPS
ATOM	849 850	C	GLU	108	-1.788	6.517	62.858	1.00 10.37	ACPS
ATOM		0	GLU	108	-0.769	7.193	62.977	1.00 10.85	ACPS
MOTA MOTA	851 852	N	TYR	109	-2.292	6.164	61.676	1.00 10.03	ACPS
ATOM	852 853	CA.	TYR	109	-1.608	6.482	60.421	1.00 9.03	ACPS
	854	CB	TYR	109	-1.061	5.195	59.757	1.00 10.14	ACPS
ATOM	855	CG	TYR	109	-0.074	4.364	60.537	1.00 9.25	ACPS
MOTA		CD1		109	1.091	4.927	61.043	1.00 9.05	ACPS
ATOM ATOM	856 857	CEI		109	2.032	4.157	61.725	1.00 10.07	ACPS
	858	CD2		109	-0.283	2.996	60.730	1.00 10.49	ACPS
ATOM		CE2		109		2.996	61.410	1.00 10.01	ACPS
ATOM	859	CEZ	TYR	109	0.649 1.807	2.217	61.902	1.00 10.01	ACPS
ATOM	860	OH	TYR	109	2.753	2.809	62.546	1.00 11.45	ACPS
ATOM	861		TYR	109			59.343	1.00 9.01	ACPS
ATOM	862	C	TYR	109	-2.487	7.101	59.343	1.00 9.80	ACPS
ATOM	863	и	ALA		-3.708	6.991	58.381	1.00 9.15	ACPS
ATOM	864	N	ΑЦΑ	110	-1.825	7.735	30.361	2.00 7.13	crb



SEP 0 9 2002

TECH CENTER 1600/2900



ATOM	865	CA	ALA	110	-2.475	8.207	57.162	1.00 10.18	ACPS
ATOM	866	CB	ALA	110	-2.489	9.726	57.072	1.00 9.95	ACPS
ATOM	867	С	ALA	110	-1.529	7.598	56.110	1.00 8.99	ACPS
ATOM	868	0	ALA	110	-0.322	7.843	56.143	1.00 10.23	ACPS ACPS
ATOM	869	N	ALA	111	-2.067	6.776	55.209	1.00 9.06	
ATOM	870	CA	ALA	111	-1.255	6.109	54.181	1.00 9.24	ACPS
ATOM	871	CB	ALA	111	-1.319	4.577	54.371	1.00 9.27	ACPS
ATOM	872	С	ALA	111	-1.710	6.462	52.773	1.00 9.10	ACPS
ATOM	873	0	ALA	111	-2.877	6.780	52.551	1.00 9.14	ACPS
ATOM	874	N	ALA	112	-0.782	6.399	51.822	1.00 9.52	ACPS
ATOM	875	CA	ALA	112	-1.107	6.713	50.434	1.00 9.40	ACPS
ATOM	876	CB	ALA	112	-0.973	8.219	50.190	1.00 10.40	ACPS
ATOM	877	С	ALA	112	-0.202	5.984	49.462	1.00 9.11	ACPS
ATOM	878	0	ALA	112	0.890	5.548	49.814	1.00 9.27	ACPS ACPS
MOTA	879	N	GLN	113	-0.680	5.843	48.233	1.00 10.03	
ATOM	880	CA	GLN	113	0.124	5.246	47.171	1.00 10.71	ACPS ACPS
ATOM	881	CB	GLN	113	-0.221	3.768	46.949	1.00 12.50	ACPS
ATOM	882	CG	GLN	113	-1.607	3.525	46.382	1.00 14.15	ACPS
ATOM	883	CD	GLN	113	-1.910	2.053	46.181	1.00 16.57	ACPS
ATOM	884	OE1	GLN	113	-2.978	1.699	45.686	1.00 17.95	ACPS
ATOM	885	NE2	GLN	113	-0.978	1.187	46.581	1.00 19.32	ACPS
ATOM	886	С	GLN	113	-0.088	6.047	45.884	1.00 10.42	ACPS
ATCA:	887	0	GLN	113	-1.121	6.698	45.701	1.00 11.38	ACPS
ATOM	888	N	VAL	114	0.905	5.998	45.002	1.00 10.88	ACPS
ATOM	889	CA	VAL	114	0.872	6.727	43.742	1.00 11.50	ACPS
ATOM	890	CB	VAL	114	1.770	8.002	43.834	1.00 12.48	ACPS
ATOM	891		VAL	114	1.994	8.613	42.444	1.00 12.51	ACPS
ATOM	892	CG2		114	1.144	9.013	44.779	1.00 11.66 1.00 11.78	ACPS
ATOM	893	С	VAL	114	1.409	5.888	42.589	1.00 11.78	ACPS
ATOM	894	0	VAL	114	2.295	5.055	42.772	1.00 11.30	ACPS
ATOM	895	N	VAL	115	0.839	6.099	41.405	1.00 12.10	ACPS
ATOM	896	CA	VAL	115	1.322	5.454		1.00 12.42	ACPS
ATOM	897	CB	VAL	115	0.426	4.301	39.706 38.377	1.00 14.70	ACPS
ATOM	898		VAL	115	0.957	3.778	40.736	1.00 12.57	ACPS
ATOM	899		VAL	115	0.388	3.172	39.109	1.00 12.96	ACPS
ATOM	900	С	VAL	115	1.364	6.525 7.167	38.821	1.00 13.15	ACPS
ATOM	901	0	VAL	115	0.351	6.732	38.534	1.00 13.59	ACPS
ATOM	902	N	ILE	116	2.547	7.708	37.454	1.00 15.01	ACPS
ATOM	903	CA	ILE	116	2.736 4.044	8.514	37.619	1.00 15.13	ACPS
ATOM	904	- CB	ILE	116	4.252	9.422	36.391	1.00 15.76	ACPS
ATOM	905		ILE	116	4.011	9.353	38.901	1.00 14.74	ACPS
ATOM	906		ILE	116	5.326	10.082	39.168	1.00 15.57	ACPS
MOTA	907		ILE	116	2.881	6.907	36.164	1.00 16.45	ACPS
ATOM	908	C	ILE	116	3.750	6.032	36.076	1.00 16.35	ACPS
MOTA	909	0	ILE	116	2.054	7.205	35.165	1.00 18.81	ACPS
MOTA	910	N	GLU	117	2.034	6.481	33.894	1.00 21.39	ACPS
ATOM	911	CA	GLU	117	0.760	6.363	33.245	1.00 22.18	ACPS
ATOM	912	CB	GLU	117	-0.272	5.679	34.124	1.00 23.46	ACPS
ATOM	913	CG	GLU	117	-1.560	5.358	33.391	1.00 24.48	ACPS
ATOM	914	CD	GLU	117	-1.580	4.373	32.622	1.00 25.10	ACPS
ATOM	915		GLU	117	-1.582 -2.550	6.092	33.580	1.00 25.49	ACPS
ATOM	916		GLU	117		7.186	32.938	1.00 23.33	ACPS
ATOM	917	C	GLU	117	3.097	8.367	33.101	1.00 23.55	ACPS
ATOM	918	0	GLU	117	3.386		31.943	1.00 25.38	ACPS
ATOM	919	N	ALA	118	3.596 4.516	6.460 7.055	30.979	1.00 27.43	ACPS
ATOM	920	CA	ALA	118			29.985	1.00 27.34	ACPS
ATOM	921	CB	ALA	118	4.977	6.002	23.303	1.00 27.51	

FIG. 2A-16



SEP 0 9 2002

FIG. 2A-17

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8.208 30.244 1.00 28.57 ACPS 3.841 ΔТОМ 922 C ALA 118 OTI ALA 118 2.598 8.169 30,110 1.00 29.57 ACPS ATOM 923 4.563 9.133 29.800 1.00 30.29 ACPS ATOM 924 OT2 ALA 118 1 8.184 16.571 66.146 1.00 24.49 WAT MOTA 925 n HOH 1.00 23.58 8.785 8.855 56.929 WAT 926 0 HOH 2 ATOM 3 -6.634 6.371 40.520 1.00 13.40 WAT ATOM 927 o HOH 6.588 56.334 1.00 12.56 WAT 4 6.850 ATOM 928 0 HOH -8.045 6.689 43.987 1.00 13.42 WAT HOH 5 MOTA 929 o 9.243 59.567 1.00 14.25 6 -5.322 WAT ATOM 930 0 HOH 7 6.897 46.767 1.00 10.54 WAT нон -8.408 ATOM 931 0 8.272 65.337 1.00 14.13 WAT MOTA 932 0 HOH R 0.163 9.350 40.005 1.00 16.00 WAT 9 -14.561 ATOM 933 0 нон 5.984 9,787 56.562 1.00 12.10 WAT ATOM 934 0 HOH 10 20.654 50.362 1.00 18.90 WAT 11 9.603 ATOM 935 0 HOH 9.199 12.001 56.416 1.00 20.43 WAT ATOM 936 0 HOH 12 -5.501 13.397 53.431 1.00 13.06 WAT 937 0 HOH 13 ATOM 25.961 44.622 1.00 17.37 WAT ATOM 938 0 нон 14 -2.767 15 1.460 20.979 40.473 1.00 16.78 WAT 939 0 HOH ATOM ATOM 940 0 HOH 16 -6.412 20.992 45.756 1.00 19.74 WAT 17 9.042 41.305 1.00 12.90 WAT 941 0 HOH -6.145 ATOM 18 42.670 1.00 18.93 ATOM 942 C нон -0.223 24.078 WAT 19 -7.596 19.455 37.156 1.00 19.34 WAT 943 0 HOH ATOM 944 C HOH 20 -5.063 33.496 51.266 1.00 22.07 WAT ATOM 0.933 67.571 1.00 14.90 WAT 945 a нон 21 -1.492 ATOM 1.00 23.19 ATOM 946 0 нон 22 10.843 7.091 38.836 WAT 68.706 1.00 24.82 ATOM 947 0 HOH 23 1.577 14.422 WAT 8.898 61.270 1.00 18.79 ATOM 948 0 HOH 24 -7.606 WAT 9.327 35.513 1.00 22.45 WAT ATOM 949 o HOH 25 0.081 18.339 48.365 1.00 15.49 WAT ATOM 950 0 нон 26 -6.295 1.00 21.01 19.887 66.759 WAT 951 o HOH 27 -0.673 ATOM 42.588 1.00 18.21 ATOM 952 0 HOH 28 2.234 22,708 WAT 5.790 62.516 1.00 18.49 WAT 953 0 нон 29 5.866 ATOM 15.961 36.660 1.00 18.35 WAT ATOM 954 a нон 30 0.991 9.357 38.563 1.00 20.48 WAT -6.406 ATOM 955 О HOH 31 ATOM 956 0 HOH 32 -11.957 11.623 37.352 1.00 24.33 WAT 14.434 49.725 1.00 27.42 WAT o HOH 33 -10.389 ATOM 957 ATOM 958 0 нон 34 -4.448 20.165 63.854 1.00 24.32 WAT HOH 1.450 2.725 43.903 1.00 20.38 WAT ATOM 959 0 35 0 HOH 36 -9.847 19.977 43.739 1.00 23.75 WAT ATOM 960 1.00 20.66 o HOH 37 -4.274 35.006 45.404 WAT ATOM 961 MOTA 962 ٥ нон 38 -0.833 22.659 40.326 1.00 19.80 WAT 39 -10.345 18.568 67.239 1.00 20.80 WAT ATOM 963 n HOH ATOM 964 o нон 40 -8.477 13.551 55.975 1.00 26.24 WAT -5.655 29.371 49.873 1.00 28.51 WAT MOTA 965 o HOH 41 966 o HOH 42 -10.675 16.934 50.659 1.00 24.92 WAT ATOM 1.00 27.30 o HOH -12.936 12.520 51.596 WAT ATOM 967 43 21.159 39.730 1.00 21.12 WAT ATOM 968 n HOH 44 5.317 1.00 26.54 o нон -16.788 9.865 48.461 WAT ATOM 969 45 970 o нон 46 -11.077 6.886 57.927 1.00 23.02 WAT ATOM 1.00 34.53 WAT ATOM 971 0 HOH 47 8.239 21.236 62.377 51.577 1.00 21.86 WAT ATOM 972 0 HOH 48 -12.230 29,900 1.00 23.96 WAT ATOM 973 a HOH 49 14.440 16.080 45.556 WAT ATOM 974 o нон 50 12.861 21.772 39.431 1.00 30.68 975 ٥ HOH 51 -14.091 19.163 60.526 1.00 27.55 WAT ATOM WAT ATOM 976 ٥ нон 52 6.663 27.800 61.179 1,00 32.84 977 o нон -11.635 27.871 53.345 1.00 31.03 WAT ATOM 53 ATOM 978 нон -6.997 7.591 67.044 1.00 25.57 WAT



TECH CENTER 1600/2900

SEP 0 9 2002



FIG. 2A-18

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ATOM	9 79	0	нон	55	5.799	6.629	59.843	1.00 16.31	WAT
ATOM	980	ō	нон	56	2.012	25.703	66.142	1.00 35.32	WAT
ATOM	981	ō	нон	57	0.121	2.727	31.610	1.00 42.03	WAT
ATOM	982	o	нон	58	1.534	10.328	32.415	1.00 41.42	WAT
ATOM	983	0	HOH	59	-16.524	4.165	56.298	1.00 21.92	WAT
ATOM	984	o	нон	60	-13.305	16.632	64.615	1.00 23.56	WAT
ATOM	985	0	HOH	61	-12.177	16.550	67.442	1.00 20.64	WAT
ATOM	986	0	нон	62	-14.009	9. 9 85	52.284	1.00 25.38	WAT
ATOM	987	0	HOH	63	-9. 9 0 0	9.225	59.680	1.00 23.49	WAT
ATOM	988	0	HOH	64	-6.771	33.311	45.569	1.00 21.83	WAT
ATOM	989	0	HOH	65	-2.713	20.087	61.546	1.00 24.39	WAT
ATOM	990	0	HOH	66	-7.980	17.897	68.615	1.00 22.87	WAT
MOTA	991	0	нон	67	-13.405	7.809	38.191	1.00 26.90	WAT
MOTA	992	0	HOH	68	-4.952	28.402	44.638	1.00 33.63	WAT
ATOM	993	0	нон	69	-2.685	3.686	68.288	1.00 31.25	WAT
ATOM	994	0	нон	70	8.512	9.048	60.830	1.00 28.65	TAW TAW
MOTA	995	0	нон	71	-1.486	18.163	62.740 70.084	1.00 32.45 1.00 26.38	WAT
MOTA	996	0	нон	72	5.603	18.678		1.00 29.41	WAT
MOTA	997	0	HOH	73	-7.547	29.689	51.621 52.981	1.00 26.05	WAT
MOTA	998	0	HOH	74	10.855 -11.689	19.331	61.337	1.00 28.03	WAT
ATOM	999	0	нон	75		23.981	38.303	1.00 33.92	WAT
MOTA	1000	0	HOH	76 77	-0.166 -11.224	22.643	66.111	1.00 30.50	WAT
MOTA	1001	0	HOH	78	15.942	18.609	39.466	1.00 35.09	WAT
ATOM	1002	0	нон	78 79	-9.721	15.254	57.360	1.00 23.81	WAT
MOTA	1003	0	нон	80	-9.623	11.467	57.685	1.00 26.57	WAT
MOTA	1004	0	HOH	81	-10.600	4.395	59.079	1.00 26.62	WAT
ATOM	1005	o	нон	82	-8.498	10.896	38.078	1.00 35.64	WAT
MOTA MOTA	1000	Ö	нон	83	-2.753	18.652	65.536	1.00 26.51	WAT
ATOM	1007	ö	нон	84	9.568	24.455	43.921	1.00 31.56	WAT
ATOM	1009	o	нон	85	19.835	12.684	45.040	1.00 35.96	WAT
ATOM	1010	ŏ	нон	86	13.338	21.812	46.003	1.00 39.76	WAT
ATOM	1011	ō	нон	87	11.096	20.032	59.974	1.00 34.99	WAT
ATOM	1012	ō	нон	88	3.720	23.855	40.646	1.00 31.59	WAT
ATOM	1013	ō	нон	89	-1.224	22.461	66.261	1.00 34.76	WAT
ATOM	1014	0	нон	90	-7.691	9.770	63.766	1.00 31.45	WAT
ATOM	1015	0	нон	91	17.406	11.773	44.998	1.00 29.99	WAT
ATOM	1016	0	нон	92	-1.506	7.951	67. 5 87	1.00 28.61	WAT
ATOM	1017	0	HOH	93	-3.462	10.383	67. 429	1.00 32.97	WAT
ATOM	1018	0	нон	94	-2.310	12.680	66.265	1.00 27.88	TAW
ATOM	1019	0	HOH	95	-4.2 9 9	16.505	66.744	1.00 34.32	WAT
ATOM	1020	0	HOH	96	0.990	24.911	62.972	1.00 31.02	TAW
MOTA	1021	0	нон	97	-13.635	13.854	63.282	1.00 15.69	WAT
MOTA	1022	0	нон	98	-12.4 72	13.178	48.835	1.00 25.84	WAT
ATOM	1023	0	HOH	99	0.796	0.192	42.865	1.00 28.22	WAT
MOTA	1024	N1	COA	120	-12.948	7.608	44.920	1.00 13.13	COA
MOTA	1025	C2	COA	120	-11.643	7.336	45.414	1.00 12.29	COA
ATOM	1026	И3	COA	120	-11.182	7.731	46.667	1.00 13.13	COA
MOTA	1027	C4	COA	120	-12.090	8.415	47.420	1.00 12.87	COA
ATOM	1028	C5	COA	120	-13.461	8.771	47.064	1.00 12.68	COA
ATOM	1029	C6	COA	120	-13.899	8.321	45.698	1.00 13.32	
ATOM	1030	N6	COA	120	-15.094	8.573	45.246	1.00 13.97	COA
ATOM	1031	N7	COA	120	-14.087	9.450	48.042	1.00 13.45	COA
ATOM	1032	C8	COA	120	-13.179	9.555	49.021	1.00 14.05	COA
ATOM	1033	И9	COA	120	-11.940	8.949	48.707	1.00 12.82	COA
ATOM	1034		COA	120	-10.508	8.739	49.433	1.00 12.92	COA
ATOM	1035	C2*	COA	120	-10.131	10.063	49.988	1.00 12.61	COA



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FIG. 2A-19

ATOM	1036		COA	120	-8.885	10.585	49.617	1.00 13.09	COA
ATOM	1037	C3 *	COA	120	-10.321	9.967	51.470	1.00 12.95	COA
ATOM	1038		COA	120	-9.269	10.478	52.488	1.00 12.93	COA
ATOM	1039	P3*	COA	120	-9.182	12.127	52.589	1.00 13.47	COA
ATOM	1040	07	COA	120	-8.835	12.768	51.184	1.00 13.51	COA
ATOM	1041	08	COA	120	-8.049	12.448	53.626	1.00 13.28	COA
ATOM	1042	09	COA	120	-10.609	12.596	53.131	1.00 14.44	COA
ATOM	1043		COA	120	-10.208	8.375	51.725	1.00 13.08	COA
ATOM	1044		COA	120	-10.977	7.897	50.509	1.00 12.26	COA
ATOM	1045		COA	120	-10.401	7.949	53.127	1.00 14.58	COA
ATOM	1046	05*	COA	120	-10.469	6.473	52.938	1.00 13.48	COA
ATOM	1047	P1	COA	120	-10.652	5.672	54.364	1.00 12.56	COA
ATOM	1048	01	COA	120	-9.729	6.240	55.365	1.00 13.21	COA
ATOM	1049	02	COA	120	-10.459	4.226	54.119	1.00 15.04	COA
ATOM	1050	03	COA	120	-12.029	6.083	54.854	1.00 16.52	COA
ATOM	1051	P2	COA	120	-13.553	5.541	54.845	1.00 22.65	COA
MOTA	1052	04	COA	120	-13.663	4.249	55.488	1.00 23.91	COA
ATOM	1053	05	COA	120	-14.429	6.530	55.551	1.00 25.17	COA
ATOM	1054	06	COA	120	-13.926	5.591	53.277	1.00 23.32	COA
ATOM	1055		COA	120	-14.755	4.650	51.149	1.00 25.32	COA
ATOM	1056		COA	120	-13.824	4.473	52.426	1.00 24.46	COA
ATOM	1057		COA	120	-14.105	5.689	50.154	1.00 25.05	COA
ATOM	1058		COA	120	-14.799	3.243	50.564	1.00 25.09	COA
ATOM	1059		COA	120	-16.252	5.244	51.556	1.00 26.37	COA
ATOM	1060		COA	120	-17.086	5.395	50.361	1.00 26.75	COA
ATOM	1061	C9	COA	120	-17.067	4.353	52.553	1.00 27.72	
ATOM	1062		COA	120	-16.649	4.199	53.819	1.00 28.04	COA
ATOM	1063	NB	COA	120	-18.144	3.780	52.101	1.00 30.34	COA
ATOM	1064	C7	COA	120	-19.329	3.490	52.916 53.477	1.00 32.23 1.00 33.78	COA
MOTA	1065		COA	120	-19.224	2.064	54.888	1.00 33.78	COA
MOTA	1066		COA	120	-19.805	1.971 2.967	55.487	1.00 34.88	COA
ATOM	1067		COA	120	-20.414		55.446	1.00 36.24	COA
MOTA	1068	N4	COA	120	-19.632	0.789	56.852	1.00 34.64	COA
MOTA	1069	C3	COA	120	-20.112	0.432	57.112	1.00 34.47	COA
ATOM	1070		COA	120	-19.736	-0.998	56.301	1.00 34.47	COA
ATOM	1071	S1	COA	120	-20.877	-2.208		1.00 33.46	IONS
ATOM		CA+2		1	7.365	8.523	54.928	1.00 11.64	IONS
ATOM		CL-1		2	5.841	9.868	59.601		IONS
ATOM	1074	CA+2	CA2	3	0.000	0.000	65.920	0.33 1.00	10142
END									



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APPROVED 5Y RAFTSMAW



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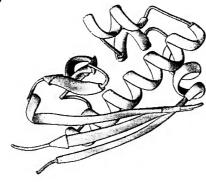
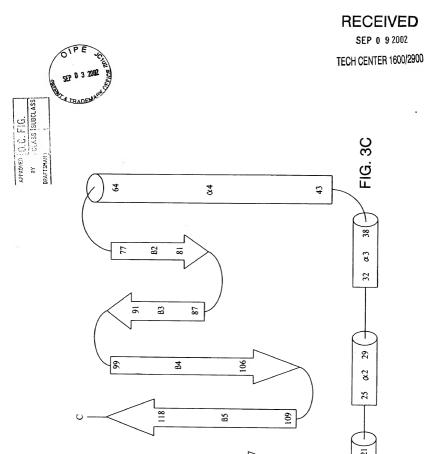


FIG. 3B



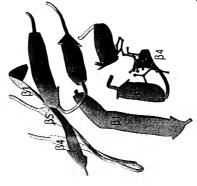


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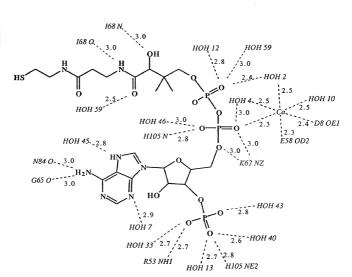


FIG. 5



JAMSS SUBCLASS

DRAFTSMAH

0.00

Residuals

0.04

-0.05-

-0.04

0.4-

Absorbance

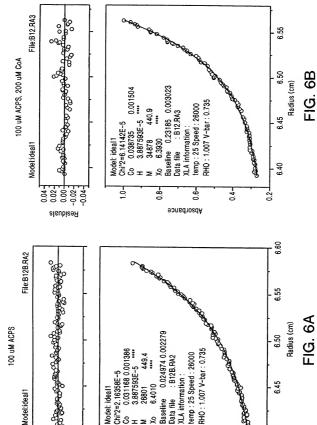
APPROVED . 0. G. F.1G.

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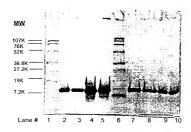


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SUBCLASS APPROVED [0, G. DRAFTSMAN

15% Non-reducing, denaturing gel of ACPS samples before and after analytical centrifugation



Lane # ACPS samples

- pH 5.2 2 3
 - pH 5.2, heated 10 min at 100 deg in gel sample buffer
- 4 pH 6.4, after sedimentation equilibrium expt.
- 5 pH 6.4, after equilibrium expt, heated 10 min at 100deg in gel buffer pH 7.4 7
- 8
 - pH 7.4, heated 10 min at 100 deg in gel buffer
- 9 pH 6.4
- 10 pH 6.4, heated 10 min at 100 deg in gel sample buffer

Lanes 2, 3, 7, 8, 9, 10: 20 uL of a freshly prepared 32 ujM ACPS sample was added Lanes 4, 5: 20 uL of the 100 uM ACPS pH 6.4 solution from the sedimentation equilbrium experiment was used

FIG. 7



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MIYGI GLDIT ELKRI ASMAG RQKRF AERIL TRSEL DQYYE LSEKR KNEFL AGRFA AKEAF SKAFG TGIGR QLSFQ DIEIR KDQNG KPYII CTKLS QAAVH VSITH TKEYA AAQVV IERLS S

FIG. 8



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Staphylococcus

Thermotoga Excherichia Rickettsia Streptomyces Treponema Bacillus Bradyrhizobium Mycobacterium consensus 150

CLASS ISUBCLASS Aquifex ----MIGVDIVKNERIKDALERFGDKFLDRIYTKRELEYCY----AHCDFLPCLAARWAG Chlamydophila MEIIHIGTDIIEISRIREAIATHGNRLLNRIFTEAEOKYCL----EKTDPIPSFAGRFAG Helicobacter ----MIGIDIVSIARIEKCVKRFKMKFLERFLSPSEIVLCK----DKSS---SIAGFFAL 1 -MIHGIGVDLIEIDRIOALYSKQ-PKLVERILTKNEOHKFNN-FTHEORKIEFLAGRFAT Staphylococcus -MIVGVGIDVLEVERVP-----EKFAERILGESEKRLF---LTRKRRR-EFIAGRFAL Thermotoga Escherichia MAILGLGTDIVEIARIEAVIARSGDRLARRVLSDNEWAIWK---THHOPV-RFLAKRFAY Rickettsia -MLIGVGTDIVOIPRIEKILNIYOELFAKKILALKELKOFT--LLNKTNHATFLAKRFSA MSIIGVGIDVAEVERFGA-ALERTPALAGRLFLESELLLP----GGERRGVASLAARFAA Streptomyces Treponema -MIIGVGIDIVEIERFVS-WTHNVRLLR-RFFHQEEIVDF----FKNHMRAQFLATRFAA Bacillus 1 -MIYGIGLDITELKRIAS-MAGRQKRFAERILTRSELDQYY--ELSEKRKNEFLAGRFAA Bradyrhizobium -MIIGIGSDLIDITRVGKVIERHGERFLDRIFTAAERAKAERRAKNEKMVVATYAKRFAA Mycobacterium MGIVGVGIDLVSIPDFAEOVSOPGTVFM-TIFTPGERRDAS---VKSSSAVCHLAARWAV G D consensus KEAVLKAFYTEFKIFL-----RFKEIEILGNRGRPPTVVINRE--GVEEILKNY----E Aquifex 53 Chlamydophila KEAVAKALGTGIGSVV-----AWKDIEVFKVSHGPEVLLPS----HVYAKIGIS----K 57 Helicobacter 50 KEACSKALOVGIGKEL-----SFLDIKISKSPKNAPLITLSK---EKMDYFNIO----S Staphylococcus KEAFSKALGTGLGKHV-----AFNDIDCYNDELGKPKI------DYEGF----I KEAFFKALGTGLNGH-----SFTDVEFLESN-GKPVLCVH-----KDFGFFN----Y Thermotoga 49 KEAAAKAFGTGIRNGL----AFNQFEVFNDELGKPRLRLWGEALKLAEKLGVA----N Escherichia 57 Rickettsia 58 KEAVSKAFGVGIGRGI-----NFKDITILNDNLGKPTVEISS---HYTNKLAPF----N KEALAKALGAPAG--L----LWTDAEVWVEAGGRPRLRVTGTVAARAAELGVA----S Streptomyces 56 Treponema 54 KEAFGKALGTGLRN-M-----ELRNIRVCONGWGKPRLEVYGAAQAMLAATGGT----H 57 KEAFSKAFGTGIGROL-----SFODIEIRKDONGKPYIICT------KLSOA----A Bacillus KEACSKALGTGIRRGV------WWRDMGVVNLPGGRPTMQLTGGALARLQALTPDGFEAR Bradyrhizobium KEAVIKAWSGSRFAORPMLPENIHRDIEVVNDMWGRPRVRLTG---AIAKHLTDV----T Mycobacterium 61 consensus 61 61......70......80.......90.......100......110...... VIVSLSHERDYSVAVAYIKKKS------101 Aquifex Chlamydophila 103 VII.SISHCKEYATATAIALA------LSASISHDAGFAIAVVVVSSSNE-----97 Helicobacter VHVSISHTEHYAMSQVVLEK------SAF-----Staphylococcus 97 Thermotoga 91 AHVSLSH-DRFAVALVVLEKRKGDIIVEGDESFLRKRFEVLERSVEGWEIETSLPPFTLK Escherichia 107 MHVTLADERHYACATVIIES-----IHLSLSDDYPICIAFAIIESNC-----105 Rickettsia WHVSLSHDAGIASAVVIAEG-----104 Streptomyces IOVSLTHEREVASAIVIIEGEPL-----Treponema 103 VHVSITHTKEYAAAQVVIERLSS-----Cacillus 99 IDVSITDDWPLAQAFVIISAVPLAKS-----Bradyrhizobium 114 Mycobacterium 110 THYSLTHEGDIAAAVVILEVI.----consensus 121......130.......140.......150.......160.......170....... 121 Aquifex Chlamydophila Helicobacter

KLLESSGCRLVRYGNILIGE

181......190......